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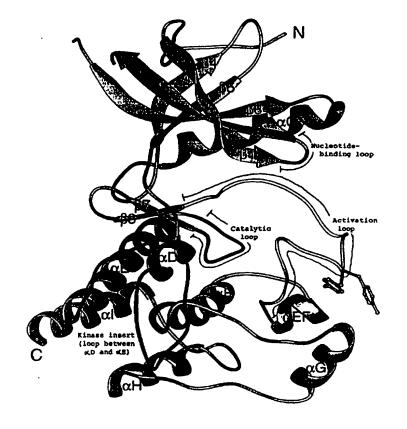
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#### (57) Abstract

The present invention relates to the threedimensional structures of a protein tyrosine kinase optionally complexed with one or more compounds. The atomic coordinates that define the structures of the protein tyrosine kinase and any of the compounds bound to it are pertinent to methods for determining the three-dimensional structures of protein tyrosine kinases with unknown structure and to methods that identify modulators of protein tyrosine kinase functions.



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#### DESCRIPTION

# CRYSTAL STRUCTURES OF A PROTEIN TYROSINE KINASE

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# RELATED APPLICATIONS

This application is related to U.S. Application Serial No. 08/701,191, by Mohammadi, et al., entitled "Crystals of the Tyrosine Kinase Domain of Non-Insulin Receptor Tyrosine Kinases," filed August 21, 1996 (Lyon & Lyon Docket No. 227/088) and U.S. Application Serial No. 60/034,168, by McMahon, et al., entitled "Crystal Structures of a Protein Tyrosine Kinase Complexed with Compounds of the Oxindolinone/Thiolindolinone Family," filed December 19, 1996 (Lyon & Lyon Docket No. 221/282), which are hereby incorporated herein by reference in their entirety including any drawings,

15 tables, and figures.

### INTRODUCTION

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The present invention relates to the three dimensional structures of protein kinases.

# BACKGROUND OF THE INVENTION

The following description of the background of the invention is provided simply as an aid in understanding 25 the invention and is not admitted to describe or constitute prior art to the invention.

Protein tyrosine kinases (PTKs) comprise a large and diverse class of enzymes (for a review, see Schlessinger and Ullrich, 1992, Neuron 9: 383-391). PTK family contains multiple subfamilies, one of which

is the fibroblast growth factor receptor (FGF-R) subfamily (for a review, see Givol and Yayon, 1992, FASEB J. 6 (15): 3362-3369).

All PTKs enzymatically transfer a high energy phosphate from adenosine triphosphate to a tyrosine 5 residue in a target protein. These phosphorylation events regulate cellular phenomena in signal transduction processes. Cellular signal transduction processes contain multiple steps that convert an extracellular signal into an intracellular signal. 10 intracellular signal is then converted into a cellular response. PTKs are components in many signal transduction processes. A PTK regulates the flow of a signal in a particular step in the process by phosphorylating a downstream molecule. The addition of 15 a phosphate can either modulate the activity of the downstream molecule by turning it "on" or "off". Thus, aberrations in a particular PTK's activity can either cause overflow or underflow of the signal. Overflow of a signal can lead to such abnormalities as uncontrolled 20 cell proliferation, which is representative of such disorders as cancer and angiogenesis.

Scientists in the biomedical community are searching for PTK inhibitors that down-regulate overflow signal transduction pathways. In particular, small molecule PTK inhibitors are sought that can traverse the cell membrane and not become hydrolyzed in acidic environments. These small molecule PTK inhibitors can be highly bioavailable and can be administered orally to patients.

Some small molecule PTK inhibitors have already

been discovered. For example, bis(monocyclic), bicyclic or heterocyclic aryl compounds (PCT WO 92/20642), vinylene-azaindole derivatives (PCT WO 94/14808), 1-cyclopropyl-4-pyridyl-quinolones (U.S. Patent No. 5,330,992), styryl compounds (U.S. Patent No. 5,217,999), styryl-substituted pyridyl compounds (U.S. Patent No. 5,302,606), certain quinazoline derivatives (EP Application No. 0 566 266 Al), seleoindoles and selenides (PCT WO 94/03427), tricyclic polyhydroxylic compounds (PCT WO 92/21660), and benzylphosphonic acid compounds (PCT WO 91/15495) are described as PTK inhibitors.

Although many PTK inhibitors are known, many of these are not specific for PTK subfamilies and will therefore cause multiple side-effects as therapeutics. Compounds of the indolinone family, however, are specific for the FGFR subfamily and are non-hydrolyzable. WO 96/40116, "Indolinone Compounds for the Treatment of Disease," published December 19, 1996, inventors Tang et al. Although the use of X-ray crystallography has provided three dimensional structures of other PTKs, they are not complexed with PTK subfamily specific, hydrolysis resistant, small molecules.

Despite recent advances, the need remains in the art for crystallographic analysis of protein kinases, so that improved therapeutic molecules can be designed and synthesized.

#### 30 SUMMARY OF THE INVENTION

The present invention relates to the three

dimensional structures of protein tyrosine kinases. The use of X-ray crystallography can define the three dimensional structure of protein tyrosine kinase at atomic resolution.

5 The three dimensional structures described herein elucidate specific interactions between protein tyrosine kinases and compounds bound to them. The coordinates that define the three dimensional structures of protein tyrosine kinases are useful for determining three dimensional structures of PTKs with unknown structure. 10 In addition, the coordinates are also useful for designing and identifying modulators of protein tyrosine kinase function. These modulators are potentially useful as therapeutics for diseases, including (but limited to) cell proliferative diseases, such as cancer, 15 angiogenesis, atherosclerosis, and arthritis.

Thus in a first aspect, the invention features a crystalline form of a polypeptide corresponding to the catalytic domain of a protein tyrosine kinase.

The term "crystalline form," in the context of the invention, is a crystal formed from an aqueous solution comprising a purified polypeptide corresponding to the catalytic domain of a PTK. A crystalline form of a protein tyrosine kinase is characterized as being capable of diffracting x-rays in a pattern defined by one of the crystal forms depicted in Blundel et al., 1976, Protein Crystallography, Academic Press. A crystalline form of a protein kinase is not characterized as being capable of diffracting x-rays in a pattern analogous to a crystalline form consisting of primarily salt or primarily a compound, for example.

The term "protein tyrosine kinase," or PTK, refers to an enzyme that transfers the high energy phosphate of adenosine triphosphate to a tyrosine residue located on a protein target.

A protein tyrosine kinase catalytic domain of the invention can originate from receptor protein tyrosine kinases that bind fibroblast growth factor (FGF). These protein tyrosine kinases are known as "FGFR" herein, and can relate to one member of the FGFR family, such as FGFR1.

The term "catalytic domain" refers to the region of a protein that can exist as a separate entity from the protein. The catalytic domain of a protein tyrosine kinase is characterized as having considerable amino acid identity to the catalytic domain of other protein tyrosine kinases. Considerable amino acid identity preferably refers to at least 30% identity, more preferably at least 35% identity, and most preferably at least 40% identity. These degrees of amino acid identity refer to the identity between different protein tyrosine kinase families. Amino acid identity for members of a given protein tyrosine kinase family range from 55% to 90%. The catalytic domain may be functional as a separate entity. The catalytic domain of a protein tyrosine kinase is also characterized as a polypeptide that is soluble in solution.

The term "identity" identity as used herein refers to a property of sequences that measures their similarity or relationship. Identity is measured by dividing the number of identical residues in the two sequences by the total number of residues and

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multiplying the product by 100. Thus, two copies of exactly the same sequence have 100% identity, but sequences that are less highly conserved and have deletions, additions, or replacements have a lower degree of identity. Those skilled in the art will recognize that several computer programs are available for determining sequence identity.

The term "functional" refers to the ability of a catalytic domain to convert a substrate into a product by phosphorylating the substrate. The term "functional" also relates to the ability of a catalytic domain to bind natural binding partners. The catalytic region may comprise an N-terminal tail, a catalytic core, and a C-terminal tail. The catalytic core is a polypeptide that can be functional in terms of catalysis. N- and C-terminal tails are polypeptide regions that may not confer appreciable functionality in terms of catalysis, but may confer functionality in terms of modulator specificity.

A polypeptide can exist as a catalytic domain eventhough it is not functional. For example, a polypeptide corresponding to a catalytic domain may not be functional if it does not harbor phosphate moieties in key areas. Multiple examples of phosphorylationstate dependent function are well documented in the art. Therefore, a catalytic domain can also exist without being functional. A measure of a protein kinase catalytic domain is a polypeptide that is homologous to other protein kinase catalytic domains.

The term "polypeptide" refers to an amino acid chain representing a portion of, or the entire sequence

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of, amino acids comprising a protein.

A preferred embodiment of the invention includes a crystalline form of a PTK that is a receptor PTK.

Receptors are proteins that straddle the inside and outside of the cell membrane. Receptor PTKs comprise an extracellular region, a transmembrane region, and an intracellular region comprising a catalytic domain.

Another preferred embodiment of the invention is the crystalline form of a receptor PTK selected from the group consisting of FGF-R, PDGF-R, FLK, CCK4, MET, TRKA, AXL, TIE, EPH, RYK, DDR, ROS, RET, LTK, ROR1, and MUSK.

Yet another preferred embodiment of the invention is the crystalline form of a PTK that is a non-receptor PTK. Non-receptor PTKs are located inside the cell and do not harbor extracellular or membrane-spanning polypeptides attached to the polypeptide corresponding to the catalytic domain. Non-receptor PTKs may harbor fatty acids or lipids, which can impart a membrane associated character to a PTK. In preferred embodiments of the invention, crystalline forms of non-receptor PTKs are selected from the group consisting of SRC, BRK, BTK, CSK, ABL, ZAP70, FES, FAK, JAK, and ACK.

In still another preferred embodiment, the invention features a crystalline form of a PTK that comprises a heavy metal atom. These types of crystals can be referred to as derivative crystals.

The term "derivative crystal" refers to a crystal where the polypeptide is in association with one or more heavy-metal atoms.

The term "association" refers to a condition of proximity between a chemical entity or compound, or

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portions or fragments thereof, and tyrosine kinase domain protein, or portions or fragments thereof. The association may be non-covalent, i.e., where the juxtaposition is energetically favored by, e.g., hydrogen-bonding, van der Waals, electrostatic or hydrophobic interactions, or it may be covalent.

The term "heavy metal atom" refers to an atom that is a transition element, a lanthanide metal, or an actinide metal. Lanthanide metals include elements with atomic numbers between 57 and 71, inclusive. Actinide metals include elements with atomic numbers between 89 and 103, inclusive.

In a preferred embodiment, the invention features a crystal of an FGF receptor tyrosine kinase domain protein. The FGF receptor tyrosine kinase domain protein can relate to FGFR1

The term "FGFR1" refers to one member of multiple receptor PTKs that are homologous to one another and bind FGF. In this context, the term "homologous" refers to at least 70% amino acid identity between two members of the FGFR family.

The term "FGFR1" can also refer to a mutant of human FGFR1 which is characterized by the amino acid sequence of SEQ ID NO:2. As compared to human FGFR1, FGFR1 contains the following amino acid substitutions: Cys-488 - Ala, Cys-584 - Ser, Leu-457 - Val, and has an additional five amino acid residues at the N-terminus (Ser-Ala-Ala-Gly-Thr).

The term "human FGFR1" refers to the tyrosine

kinase domain of human fibroblast growth factor receptor

("FGFR1") having the amino acid sequence of SEQ ID

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NO:1. Generally, human FGFR1 comprises a 310 amino acid residue fragment (residues 456 to 765) of human FGFR1.

The term "mutant" refers to a polypeptide which is obtained by replacing at least one amino acid residue in a native tyrosine kinase domain with a different amino acid residue. Mutation can be accomplished by adding and/or deleting amino acid residues within the native polypeptide or at the N- and/or C-terminus of a polypeptide corresponding to a native tyrosine kinase domain having substantially the same three-dimensional structure as the native tyrosine kinase domain from which it is derived. By having substantially the same three-dimensional structure is meant having a set of atomic structure coordinates that have a root mean square deviation (r.m.s.d.) of less than or equal to about 2 Å when superimposed with the atomic structure coordinates of the native tyrosine kinase domain from which the mutant is derived when at least about 50% to 100% of the  $C\alpha$  atoms of the native tyrosine kinase are included in the superposition. A mutant may have, but need not have, PTK activity.

In another preferred embodiment, the invention relates to a crystalline form defined by the structural coordinates set forth in Table 1.

25 The term "atomic structural coordinates" as used herein refers to a data set that defines the three dimensional structure of a molecule or molecules.

Structural coordinates can be slightly modified and still render nearly identical three dimensional

30 structures. A measure of a unique set of structural coordinates is the root-mean-square deviation of the

resulting structure. Structural coordinates that render three dimensional structures that deviate from one another by a root-mean-square deviation of less than 1.5 Å may be viewed by a person of ordinary skill in the art as identical. Hence, the structural coordinates set forth in Table 1, Table 2, Table 3, and Table 4 are not limited to the values defined therein.

In other preferred embodiments, the invention features a crystalline form of the polypeptide in

association with a compound. These types of crystalline forms can be referred to as co-crystals. The compound may be a cofactor, substrate, substrate analog, inhibitor, or allosteric effector.

The term "compound" refers to an organic molecule.

The term "organic molecule" refers to a molecule which has at least one carbon atom in its structure. The compound can have a molecular weight of less than 6kDa. Both the geometry of the compound and the interactions formed between the compound and the polypeptide

preferably govern high affinity binding between the two molecules. High affinity binding is preferably governed by a dissociation equilibrium constant on the order of 10-6 M or less. The compound is preferably a modulator that alters the function of a PTK.

The term "function," in reference to the effect of a modulator on PTK function, refers to the ability of a modulator to enhance or inhibit the catalytic activity of a PTK.

The term "catalytic activity", in the context of
the invention, defines the ability of a PTK to
phosphorylate a substrate polypeptide. Catalytic



activity can be measured, for example, by determining the amount of a substrate converted to a product as a function of time. The conversion of the substrate to a product occurs at the active-site of the PTK.

The term "active-site" refers to a cavity located in the PTK in which one or more substrate molecules may bind. Addition of a modulator to cells expressing a PTK may enhance (activate) or lower (inhibit) the catalytic activity of the PTK.

A small number of inhibitors of PTK catalytic activity are known in the art. Small molecule inhibitors may modulate PTK function by blocking the binding of substrates. Indolinone compounds, for example, may bind to the active-site of PTK catalytic domains and inhibit them effectively, as measured by inhibition constants on the order of 10.6 M or less.

Activators of PTK intracellular regions can enhance PTK function by interacting with both the PTK catalytic domain and the substrate. Activators may also promote dimerization of PTKs and thus activate them by bringing them into close proximity with one another. In addition, activators may operate by promoting a conformational change in the intracellular region of the PTK such that the catalytic region modifies substrates at a faster rate in the presence of the activator.

The term "function" can also refer to the ability of a modulator to enhance or inhibit the association between a PTK and a natural binding partner.

The term "natural binding partner" refers to a polypeptide that normally binds to a PTK in a cell.

These natural binding partners can play a role in

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propagating a signal in a PTK signal transduction process. The natural binding partner can bind to a PTK with high affinity. High affinity represents an equilibrium binding constant on the order of 10<sup>-6</sup> M or less. However, a natural binding partner can also transiently interact with a PTK and chemically modify it. PTK natural binding partners are chosen from a group consisting of, but not limited to, src homology 2

(SH2) or 3 (SH3) domains, other phosphoryl tyrosine binding (PTB) domains, nucleotide exchange factors, and other protein kinases or protein phosphatases.

The term "interactions" refers to hydrophobic, aromatic, and ionic forces and hydrogen bonds formed between atoms in the modulator and the enzyme activesite.

The term "cofactor" refers to a compound that may, in addition to the substrate, bind to a protein and undergo a chemical reaction. Multiple co-factors are nucleotides or nucleotide derivatives, such as phosphate and nicotinamide derivatives of adenosine.

The term "substrate" refers to a compound that reacts with an enzyme. Enzymes can catalyze a specific reaction on a specific substrate. For example, PTKs can phosphorylate specific protein and peptide substrates on tyrosine moieties. In addition, nucleotides can act as substrates for protein kinases.

The term "substrate analog" refers to a compound that is structurally similar, but not identical, to a substrate. The substrate analog may be a nucleotide analog. Examples of nucleotide analogs are described below.

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The term "inhibitor" refers to a compound that decreases the cellular function of a protein kinase. The protein kinase function is preferably the interaction with a natural binding partner and more preferably catalytic activity.

The term "allosteric effector" refers to a compound that causes allosteric interactions in a protein. The term "allosteric interactions" refers to interactions between separate sites on a protein. The sites can be different from the active site. The allosteric effector can enhance or inhibit catalytic activity by binding to a site that may be different than the active site.

The term "co-crystal" refers to a crystal where the polypeptide is in association with one or more compounds.

In preferred embodiments, a co-crystal of the invention can be in association with a heavy metal atom. Examples of heavy metal atoms are described above.

In other preferred embodiments, the invention features a co-crystal comprising the crystalline form of the polypeptide in association with a compound, where the compound is a non-hydrolyzable analog of ATP. These analogs can be referred to as nucleotide analogs.

The term "ATP" refers to the chemical compound adenosine triphosphate.

The term "non-hydrolyzable" refers to a compound having a covalent bond that does not readily react with water. Examples of non-hydrolyzable analogs of ATP are AMP-PNP and AMP-PCP, whose structures are well known to those skilled in the art.

The term "AMP-PNP" refers to adenylyl

imidodiphosphate, a non-hydrolyzable analog of ATP.

The term "AMP-PCP" refers to adenylyl diphosphonate, a non-hydrolyzable analogue of ATP.

In another preferred embodiment, the invention relates to a crystalline form defined by the structural coordinates set forth in Table 2.

In preferred embodiments, the invention relates to crystalline forms, where the compound in association with the polypeptide is an indolinone.

Certain indolinones are specific modulators of PTK function. A preferred embodiment of the invention is the crystalline form of a PTK complexed with an indolinone of formula I or II:

$$R_{5}$$
 $R_{6}$ 
 $R_{7}$ 
 $R_{1}$ 
 $R_{4}$ 
 $R_{6}$ 
 $R_{6}$ 
 $R_{7}$ 
 $R_{1}$ 
 $R_{4}$ 
 $R_{6}$ 
 $R_{6}$ 
 $R_{7}$ 
 $R_{1}$ 

or a pharmaceutically acceptable salt, isomer, metabolite, ester, amide, or prodrug thereof, where:

- (a)  $A_1$ ,  $A_2$ ,  $A_3$ , and  $A_4$  are independently carbon or nitrogen;
  - (b) R<sub>1</sub> is hydrogen or alkyl;
  - (c)  $R_2$  is oxygen in the case of an oxindolinone or sulfur in the case of a thiolindolinone;
    - (d) R<sub>3</sub> is hydrogen;
- (e) R<sub>4</sub>, R<sub>5</sub>, R<sub>6</sub>, and R<sub>7</sub> are optionally present, and are either (i) independently selected from the group consisting of alkyl, alkoxy, aryl, aryloxy, alkaryl, alkaryloxy, halogen, trihalomethyl, S(O)R, SO<sub>2</sub>NRR', SO<sub>3</sub>R, SR, NO<sub>2</sub>, NRR', OH, CN, C(O)R, OC(O)R, NHC(O)R, (CH<sub>2</sub>)<sub>n</sub>CO<sub>2</sub>R, and CONRR' or (ii) any two adjacent R<sub>4</sub>, R<sub>5</sub>, R<sub>6</sub>, and R<sub>7</sub> taken together form a fused ring with the aryl portion of the indole-based portion of the indolinone;
- (f) R<sub>2</sub>', R<sub>3</sub>', R<sub>4</sub>', R<sub>5</sub>', and R<sub>6</sub>' are each
  independently selected from the group consisting of
  hydrogen, alkyl, alkoxy, aryl, aryloxy, alkaryl,
  alkaryloxy, halogen, trihalomethyl, S(O)R, SO<sub>2</sub>NRR', SO<sub>3</sub>R,
  SR, NO<sub>2</sub>, NRR', OH, CN, C(O)R, OC(O)R, NHC(O)R, (CH<sub>2</sub>) CO<sub>2</sub>R,

and CONRR';

- (g) n is 0, 1, 2, or 3;
- (h) R is hydrogen, alkyl or aryl;
- (i) R' is hydrogen, alkyl or aryl; and
- 5 (j) A is a five membered heteroaryl ring selected from the group consisting of thiophene, pyrrole, pyrazole, imidazole, 1,2,3-triazole, 1,2,4-triazole, oxazole, isoxazole, thiazole, isothiazole, furan, 1,2,3oxadiazole, 1,2,4-oxadiazole, 1,2,5-oxadiazole, 1,3,4-
- oxadiazole, 1,2,3,4-oxatriazole, 1,2,3,5-oxatriazole, 10 1,2,3-thiadiazole, 1,2,4-thiadiazole, 1,2,5-thiadiazole, 1,3,4-thiadiazole, 1,2,3,4-thiatriazole, 1,2,3,5thiatriazole, and tetrazole, optionally substituted at one or more positions with alkyl, alkoxy, aryl, aryloxy, 15
- alkaryl, alkaryloxy, halogen, trihalomethyl, S(O)R,  $SO_2NRR'$ ,  $SO_3R$ , SR,  $NO_2$ , NRR', OH, CN, C(O)R, OC(O)R, NHC(O)R,  $(CH_2)_nCO_2R$  or CONRR'.

The term "pharmaceutically acceptable salt" refers to those salts which retain the biological activity and 20 properties of the free bases. Pharmaceutically acceptable salts can be obtained by reaction with inorganic acids such as hydrochloric acid, hydrobromic acid, sulfuric acid, nitric acid, phosphoric acid, methanesulfonic acid, ethanesulfonic acid, p-

25 toluenesulfonic acid, salicylic acid and the like.

The term "prodrug" refers to an agent that is converted into the parent drug in vivo. Prodrugs may be easier to administer than the parent drug in some situations. For example, the prodrug may be bioavailable by oral administration but the parent is not, or the prodrug may improve solubility to allow for

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intravenous administration.

"Alkyl" refers to a straight-chain, branched or cyclic saturated aliphatic hydrocarbon. Preferably, the alkyl group has 1 to 12 carbons. More preferably, it is a lower alkyl of from 1 to 7 carbons, more preferably 1 to 4 carbons. Typical alkyl groups include methyl, ethyl, propyl, isopropyl, butyl, isobutyl, tertiary butyl, pentyl, hexyl and the like. The alkyl group may be optionally substituted with one or more substituents are selected from the group consisting of hydroxyl, cyano, alkoxy, =0, =S, NO<sub>2</sub>, halogen, N(CH<sub>3</sub>)<sub>2</sub> amino, and SH.

"Alkenyl" refers to a straight-chain, branched or cyclic unsaturated hydrocarbon group containing at least one carbon-carbon double bond. Preferably, the alkenyl group has 2 to 12 carbons. More preferably it is a lower alkenyl of from 2 to 7 carbons, more preferably 2 to 4 carbons. The alkenyl group may be optionally substituted with one or more substituents selected from the group consisting of hydroxyl, cyano, alkoxy, =0, =S, NO<sub>2</sub>, halogen, N(CH<sub>3</sub>)<sub>2</sub> amino, and SH.

"Alkynyl" refers to a straight-chain, branched or cyclic unsaturated hydrocarbon containing at least one carbon-carbon triple bond. Preferably, the alkynyl group has 2 to 12 carbons. More preferably it is a lower alkynyl of from 2 to 7 carbons, more preferably 2 to 4 carbons. The alkynyl group may be optionally substituted with one or more substituents selected from the group consisting of hydroxyl, cyano, alkoxy, =0, =S, NO<sub>2</sub>, halogen, N(CH<sub>3</sub>)<sub>2</sub> amino, and SH.

"Alkoxy" refers to an "O-alkyl" group.

"Aryl" refers to an aromatic group which has at least one ring having a conjugated pi-electron system and includes carbocyclic aryl, heterocyclic aryl and biaryl groups. The aryl group may be optionally

substituted with one or more substituents selected from the group consisting of halogen, trihalomethyl, hydroxyl, SH, OH, NO<sub>2</sub>, amine, thioether, cyano, alkoxy, alkyl, and amino.

"Alkaryl" refers to an alkyl that is covalently joined to an aryl group. Preferably, the alkyl is a lower alkyl.

"Carbocyclic aryl" refers to an aryl group wherein the ring atoms are carbon.

"Heterocyclic aryl" refers to an aryl group having from 1 to 3 heteroatoms as ring atoms, the remainder of the ring atoms being carbon. Heteroatoms include oxygen, sulfur, and nitrogen. Thus, heterocyclic aryl groups include furanyl, thienyl, pyridyl, pyrrolyl, N-lower alkyl pyrrolo, pyrimidyl, pyrazinyl, imidazolyl and the like.

"Amide" refers to -C(0)-NH-R, where R is alkyl, aryl, alkylaryl or hydrogen.

"Thioamide" refers to -C(S)-NH-R, where R is alkyl, aryl, alkylaryl or hydrogen.

"Amine" refers to a -N(R')R'' group, where R' and R'' are independently selected from the group consisting of alkyl, aryl, and alkylaryl.

"Thioether" refers to -S-R, where R is alkyl, aryl, or alkylaryl.

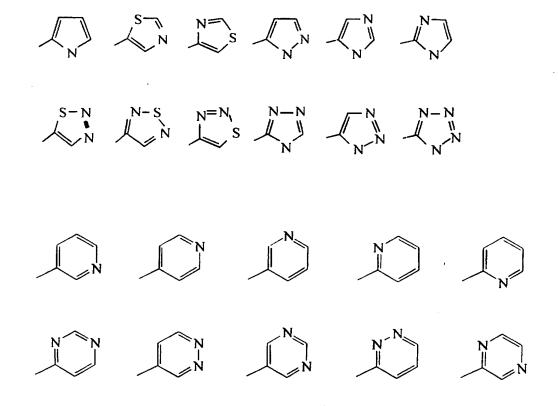
"Sulfonyl" refers to  $-S(O)_2-R$ , where R is aryl, C(CN)=C-aryl, CH<sub>2</sub>CN, alkyaryl, sulfonamide, NH-alkyl, NH-

alkylaryl, or NH-aryl.

The term "acyl" denotes groups -C(0)R, where R is alkyl as defined above, such as formyl, acetyl, propionyl, or butyryl.

It is understood by those skilled in the art that when  $A_1$ ,  $A_2$ ,  $A_3$ , and  $A_4$  are nitrogen or sulfur that the corresponding  $R_4$ ,  $R_5$ ,  $R_6$ , and  $R_7$ , as well as the corresponding bond, do not exist.

Examples of indoles having such fused rings (as described in (e) (ii) above include the following:



The six membered rings shown above exemplify possible A rings in compound II.

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Other preferred embodiments of the invention are crystalline forms comprising 3-[(3-(2-carboxyethyl)-4-methylpyrrol-5-yl)methylene]-2-indolinone as well as 3-[4-(4-formylpiperazine-1-yl-)benzylidenyl]-2-indolinone. The polypeptide of these crystalline forms can be FGFR, and specifically, FGFR1.

In preferred embodiments, the crystalline forms of the invention can be defined by the structural coordinates set forth in Table 3 or Table 4.

The use of X-ray crystallography can elucidate the three dimensional structure of crystalline forms of the invention. The first characterization of crystalline forms by X-ray crystallography can determine the unit cell shape and its orientation in the crystal.

In other preferred embodiments, the invention features a crystal of an FGF receptor tyrosine kinase domain protein, where the crystal is characterized by having monoclinic unit cells. The crystal may also be characterized by having space group symmetry C2.

The term "unit cell" refers to the smallest and simplest volume element (i.e., parallelpiped-shaped block) of a crystal that is completely representative of the unit of pattern of the crystal. The dimensions of the unit cell are defined by six numbers: dimensions a, b and c and angles  $\alpha$ ,  $\beta$  and  $\gamma$ . A crystal can be viewed as an efficiently packed array of multiple unit cells. Detailed descriptions of crystallographic terms are described in, which is hereby incorporated herein by reference in its entirety, including any drawings, figures, and tables.

The term "monoclinic unit cell" refers to a unit

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cell where a  $\neq$  b  $\neq$  c;  $\alpha = \gamma = 90^{\circ}$ ; and  $\beta > 90^{\circ}$ .

The term "space group" refers to the symmetry of a unit cell. In a space group designation (e.g., C2) the capital letter indicates the lattice type and the other symbols represent symmetry operations that can be carried out on the unit cell without changing its appearance.

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The term "lattice" in reference to crystal structures refers to the array of points defined by the vertices of packed unit cells.

The term "symmetry operations" refers to geometrically defined ways of exchanging equivalent parts of a unit cell, or exchanging equivalent molecules between two different unit cells. Examples of symmetry operations are screw axes, centers of inversion, and mirror planes.

In a preferred embodiment, the invention features a crystalline form, where the monoclinic unit cells have dimensions of about a=208.3 Å, b=57.8 Å, c=65.5 Å and  $\beta$ =107.2°.

In a preferred embodiment, the invention features a FGFR1 crystal, where the monoclinic unit cells have dimensions of about a=211.6 Å, b=51.3 Å, c=66.1 Å and  $\beta$ =107.7°.

In another aspect the invention features a polypeptide corresponding to the catalytic domain of a protein tyrosine kinase, containing at least about 20 amino acid residues upstream of the first glycine in the conserved glycine-rich region of the catalytic domain, and at least about 17 amino acid residues downstream of the conserved arginine located at the C-terminal

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boundary of the catalytic domain.

The polypeptides of the invention can be isolated, enriched or purified. In addition, the crystalline forms of the invention can be formed from polypeptides that are isolated, enriched, or purified.

By "isolated" in reference to a polypeptide is meant a polymer of 6, 12, 18 or more amino acids conjugated to each other, including polypeptides that are isolated from a natural source or that are synthesized. The isolated polypeptides of the present invention are unique in the sense that they are not found in a pure or separated state in nature. Use of the term "isolated" indicates that a naturally occurring sequence has been removed from its normal cellular environment. Thus, the sequence may be in a cell-free solution or placed in a different cellular environment. The term does not imply that the sequence is the only amino acid chain present, but that it is essentially free (about 90 - 95% pure at least) of material naturally associated with it

By the use of the term "enriched" in reference to a polypeptide it is meant that the specific amino acid sequence constitutes a significantly higher fraction (2 - 5 fold) of the total of amino acids present in the cells or solution of interest than in normal or diseased cells or in the cells from which the sequence was taken. This could be caused by a person by preferential reduction in the amount of other amino acids present, or by a preferential increase in the amount of the specific amino acid sequence of interest, or by a combination of the two. However, it should be noted that "enriched"

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does not imply that there are no other amino acid sequences present, just that the relative amount of the sequence of interest has been significantly increased. The term significant here is used to indicate that the level of increase is useful to the person making such an increase, and generally means an increase relative to other amino acids of about at least 2 fold, more preferably at least 5 to 10 fold or even more. The term also does not imply that there are no amino acids from other sources. The other source amino acids may, for example, comprise amino acids encoded by a yeast or bacterial genome, or a cloning vector such as pUC19. The term is meant to cover only those situations in which a person has intervened to elevate the proportion of the desired nucleic acid.

It is also advantageous for some purposes that an amino acid sequence be in purified form. The term "purified" in reference to a polypeptide does not require absolute purity (such as a homogeneous preparation); instead, it represents an indication that the sequence is relatively purer than in the natural environment (compared to the natural level this level should be at least 2-5 fold greater, e.g., in terms of mg/ml). Purification of at least one order of magnitude, preferably two or three orders, and more preferably four or five orders of magnitude is expressly contemplated. The substance is preferably free of contamination at a functionally significant level, for example 90%, 95%, or 99% pure.

In a preferred embodiment, the invention features a polypeptide corresponding to the catalytic domain of a

receptor PTK. The receptor PTK may have a threedimensional structure substantially similar to that of the insulin receptor, even though the amino acid content may be different.

In a preferred embodiment, the invention features a polypeptide corresponding to the catalytic domain of a non-receptor PTK, where the non-insulin receptor tyrosine kinase is a cytoplasmic tyrosine kinase.

In a preferred embodiment, the invention features a polypeptide corresponding to the catalytic domain of a receptor PTK, selected from the group consisting of FGF-R, PDGF-R, KDR, CCK4, MET, TRKA, AXL, TIE, EPH, RYK, DDR, ROS, RET, LTK, ROR1, or MUSK.

In a preferred embodiment, the invention features a polypeptide corresponding to the catalytic domain of a non-receptor PTK, selected from the group consisting of SRC, BRK, BTK, CSK, ABL, ZAP70, FES, FAK, JAK, or ACK.

In a preferred embodiment, the invention features a polypeptide corresponding to the catalytic domain of a PTK, having the amino acid sequence shown in Table 1 or Table 2.

In another aspect, the invention features a method for creating crystalline forms described herein. The method may utilize the polypeptides described herein to form a crystal. The method comprises the steps of:

- (a) mixing a volume of polypeptide solution with a reservoir solution; and
- (b) incubating the mixture obtained in step(a) over the reservoir solution in a closed container,under conditions suitable for crystallization.

These processes are described in detail in the

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section entitled "Detailed Description of the Invention."

In another aspect, the invention features a method of obtaining FGF receptor tyrosine kinase domain polypeptide in crystalline form, comprising the steps of: (a) mixing a volume of polypeptide solution with an equal volume of reservoir solution, where the polypeptide solution comprises 1 mg/mL to 60 mg/mL FGFtype tyrosine kinase domain protein, 10 mM to 200 mM buffering agent, 0 mM to 20 mM dithiothreitol and has a pH of about 5.5 to about 7.5, and where the reservoir solution comprises 10% to 30% (w/v) polyethylene glycol, 0.1 M to 0.5 M ammonium sulfate, 0% to 20% (w/v)ethylene glycol or glycerol, 10 mM to 200 mM buffering agent and has a pH of about 5.5 to about 7.5; and (b) incubating the mixture obtained in step (a) over said reservoir solution in a closed container at a temperature between 0° and 25°C until crystals form.

In a preferred embodiment, the invention features a method of obtaining FGF receptor tyrosine kinase domain polypeptide in crystalline form, where the polypeptide solution comprises about 10 mg/mL FGF receptor tyrosine kinase domain, about 10 mM sodium chloride, about 2 mM dithiothreitol, about 10 mM Tris-HCl and has a pH of about 8; the reservoir buffer comprises about 16% (w/v) polyethylene glycol (MW 10000), about 0.3 M ammonium sulfate, about 5% ethylene glycol or glycerol, about 100 mM bis-Tris and has a pH of about 6.5; and the temperature is about 4°C.

In another preferred embodiment, the invention features a method of obtaining FGF receptor tyrosine

kinase domain polypeptide in crystalline form, where the polypeptide solution includes a compound such as a cofactor, substrate, substrate analog, inhibitor or allosteric effector.

In still another preferred embodiment, the invention features a method of obtaining FGF receptor tyrosine kinase domain polypeptide in crystalline form, where the compound is a nucleotide analog, such as a non-hydrolyzable analog of ATP, or an indolinone.

Indolinone compounds have the general structural formula as described herein.

In another aspect, the invention features a cDNA encoding an FGF receptor tyrosine kinase domain protein, where a coding strand of the cDNA has the nucleotide sequence of SEQ ID NO:5.

Another aspect of the invention relates to a method of determining three dimensional structures of PTKs with unknown structure by utilizing the structural coordinates of Table 1, Table 2, Table 3, and Table 4. These methods can relate to homology modeling, molecular replacement, and nuclear magnetic resonance methods.

In a preferred embodiment, the invention relates to a method of determining three dimensional structures of PTKs with unknown structures by utilizing the coordinates of Table 1, Table 2, Table 3, or Table 4 in conjunction with the amino acid sequences of PTKs. This method of homology modeling comprises the steps of: (a) aligning the computer representation of an amino acid sequence of a PTK with unknown structure with that of a PTK with known structure, where alignment is achieved by matching homologous regions of the amino acid sequences;

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(b) transferring the computer representation of an amino acid structure in the PTK sequence of known structure to a computer representation of a structure of the corresponding amino acid in the PTK sequence with unknown structure; and (c) determining low energy conformations of the resulting PTK structure.

The term "amino acid sequence" describes the order of amino acids in the amino acid chain comprising a polypeptide corresponding to the catalytic domain of a PTK.

The term "aligning" describes matching the beginning and the end of two or more amino acid sequences. Homologous amino acid sequences are placed on top of one another during the alignment process.

The term "homologous" describes amino acids in two sequences that are identical or have similar side-chain chemical groups (e.g., aliphatic, aromatic, polar, negatively charged, or positively charged).

The term "corresponding" refers to an amino acid that is aligned with another in the sequence alignment mentioned above.

The term "determining the low energy conformation" describes a process of changing the conformation of the PTK structure such that the structure is of low free energy. The PTK structure may or may not have molecules, such as modulators bound to it.

The term "low free energy" describes a state where the molecules are in a stable state as measured by the process. A stable state is achieved when favorable interactions are formed within the complex.

The term "favorable interactions" refers to

hydrophobic, aromatic, and ionic forces, and hydrogen bonds.

Another preferred embodiment of the invention relates to a method of determining three dimensional structures of PTKs with unknown structure. This method is accomplished by applying the structural coordinates of Table 1, Table 2, Table 3, or Table 4 to an incomplete X-ray crystallographic data set for a PTK. The method comprises the steps of: (a) aligning the positions of atoms in the unit cell by matching electron diffraction data from two crystals, where one data set is complete and the other is incomplete; and (b) determining a low energy conformation of the resulting PTK structure.

The term "incomplete data set" relates to a X-ray crystallographic data set that does not have enough information to give rise to a three dimensional structure.

In another preferred embodiment, the invention relates to a method of determining three dimensional structures of PTKs with unknown structure by applying the structural coordinates of Table 1, Table 2, Table 3, or Table 4 to nuclear magnetic resonance (NMR) data of a PTK. This method comprises the steps of: (a)

determining the secondary structure of a PTK structure using NMR data; and (b) simplifying the assignment of through-space interactions of amino acids. The PTK structure may not be complexed with compounds or modulators.

The term "secondary structure" describes the arrangement of amino acids in a three dimensional

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structure, such as in  $\alpha$ -helix or  $\beta$ -sheet elements.

The term "through-space interactions" defines the orientation of the secondary structural elements in the three dimensional structure and the distances between amino acids from different portions of the amino acid sequence.

The term "assignment" defines a method of analyzing NMR data and identifying which amino acids give rise to signals in the NMR spectrum.

In another aspect, the invention features a method of identifying potential modulators of PTK function.

These modulators are identified by docking a computer representation of a structure of a compound with a computer representation of a cavity formed by the active-site of a PTK. The computer representation of the PTK active-site structure can be defined by structural coordinates.

The term "chemical group" refers to moieties that can form hydrogen bonds, hydrophobic, aromatic, or ionic interactions.

The term "docking" refers to a process of placing a compound in close proximity with a PTK. The term can also refer to a process of finding low energy conformations of the compound/PTK complex.

A preferred embodiment of the invention is a method of identifying potential modulators of PTK function.

The method involves utilizing the structural coordinates or a PTK three dimensional structure. The structural coordinates set forth in Table 1, Table 2, Table 3, and

Table 4 can be utilized. The method comprises the steps of: (a) removing a computer representation of a PTK

structure and docking a computer representation of a compound from a computer data base with a computer representation of the active-site of the PTK; (b) determining a conformation of the complex with a favorable geometric fit and favorable complementary interactions; and (c) identifying compounds that best fit the PTK active-site as potential modulators of PTK function. The initial PTK structure may or may not have compounds bound to it.

The term "favorable geometric fit" refers to a conformation of the compound-PTK complex where the surface area of the compound is in close proximity with the surface area of the active-site without forming unfavorable interactions. Unfavorable interactions can be steric hindrances between atoms in the compound and atoms in the PTK active-site.

The term "favorable complementary interactions" relates to hydrophobic, aromatic, ionic, and hydrogen bond donating, and hydrogen bond accepting forces formed between the compound and the PTK active-site.

The term "potential" qualifies the term "modulator of PTK function" because the potential modulator or PTK function has not yet been tested for activity in vitro or in vivo.

The term "best fit" describes compounds that complexed the most surface area in the complex and/or form the most favorable complementary interactions with the PTK in the screen in a given experiment.

Another preferred embodiment of the invention is a method of identifying potential modulators of PTK function. The method involves utilizing a three

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dimensional structure of a PTK, with or without compounds bound to it. The method comprises the steps of: (a) modifying a computer representation of a PTK having one or more compounds bound to it, where the computer representations of the compound or compounds and PTK are defined by structural coordinates; (b) determining a conformation of the complex with a favorable geometric fit and favorable complementary interactions; and (c) identifying the compounds that best fit the PTK active-site as potential modulators of PTK function.

The term "modifying" relates to deleting a chemical group or groups or adding a chemical group or groups.

Computer representations of the chemical groups can be selected from a computer data base.

Yet another preferred embodiment of the invention is a method of identifying potential modulators of PTK function by operating modulator construction or modulator searching computer programs on the compounds complexed with the PTK. The method comprises the steps of: (a) removing a computer representation of one or more compounds complexed with a PTK; and (b) searching a data base for compounds similar to the removed compounds using a compound searching computer program, or replacing portions of the compounds complexed with the PTK with similar chemical structures from a data base using a compound construction computer program, where the representations of the compounds are defined by structural coordinates.

The term "operating" as used herein refers to utilizing the three-dimensional conformation of

molecules defined by the processes described herein in various computer programs.

The term "similar compound" refers to a compound in a computer data base that has a similar geometric structure as compounds that can bind to a PTK. The similar compound can also have similar chemical groups as the compounds that are either bound to the PTK or once bound to the PTK. The similar chemical groups can form complementary interactions with the PTK.

The term "compound searching computer program"

describes a computer program that searches computer

representations of compounds from a computer data base
that have similar three dimensional structures and

similar chemical groups as a compound of interest. The

compound of interest is preferably an indolinone
compound.

The term "similar chemical structures" refers to chemical groups that share similar geometry as portions of the compounds in complex with the PTK or compounds removed from the PTK structure. Similar chemical structures can also refer to chemical groups that may form similar complementary interactions as portions of the compounds in complex with the PTK or compounds removed from the PTK structure.

The term "replacing structures" refers to removing a portion of the compounds in complex with the PTK or compounds removed from the PTK structure and connecting the broken bonds to a similar chemical structure.

The term "compound construction computer program"

describes a computer program that replaces computer
representations of chemical groups in a compound with

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groups from a computer data base. The compound is preferably an indolinone compound.

The term "similar three dimensional structure" describes two molecules with nearly identical shape and volume.

In another preferred embodiment of the invention, the PTK structures used in the modulator design or identification method of the invention are defined by the structural coordinates of Table 1, Table 2, Table 3, or Table 4.

The methods for using the crystalline forms and three dimensional structures of the invention can relate to a broad range of protein kinases. Thus, in preferred embodiments, the invention relates to a receptor PTK. The receptor PTK can be selected form the group consisting of FGF-R, PDGF-R, FLK, CCK4, MET, TRKA, AXL, TIE, EPH, RYK, DDR, ROS, RET, LTK, ROR1, and MUSK. The PTK may also exist as a non-receptor PTK. The non-receptor PTK can be selected from the group consisting of SRC, BRK, BTK, CSK, ABL, ZAP70, FES, FAK, JAK, and ACK.

In another aspect, the invention features a potential modulator of PTK function identified by methods disclosed in the invention.

A preferred embodiment of the invention is that the potential modulator of PTK function is an oxindolinone or a thiolindolinone of formula I or II disclosed above.

Another aspect of the invention is a method for synthesizing a potential modulator of PTK function or its pharmaceutically acceptable salts, isomers, metabolites, esters, amides, or prodrugs by a standard

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synthetic method known in the art. Synthetic procedures are discussed below.

In another aspect, the invention features a method of identifying a potential modulator of PTK function as a modulator of PTK function. The method comprises the steps of: (a) administering a potential modulator of PTK function to cells; (b) comparing the level of PTK phosphorylation between cells not administered the potential modulator and cells administered the potential modulator; and (c) identifying the potential modulator as a modulator of PTK function based on the difference in the level of PTK phosphorylation.

The term "cells" refers to any type of cells either primary or cultured. Primary cells can be extracted directly from an organism while cultured cells rapidly divide and can be cultured in many successive rounds. Cells can be grown in a variety of containers including, but not limited to flasks, dishes, and well plates.

The term "administer" refers to a method of delivering a compound to cells. The compound can be prepared using a carrier such as dimethyl sulfoxide (DMSO) in an aqueous solution. The aqueous solution comprising the compound, also termed an "aqueous preparation", can be simply mixed into the medium bathing the layer of cells or microinjected into the cells themselves. The compounds may be administered to the cells using a suitable buffered solution.

The term "suitable buffered solution" refers to an aqueous preparation of the compound that comprises a salt that can control the pH of the solution at low concentrations. Because the salt exists at low

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concentrations, the salt preferably does not alter the function of the cells.

The term "PTK phosphorylation" refers to the presence of phosphate on the PTK. Phosphates on PTKs can be identified by antibodies that bind them specifically with high affinity.

In another aspect, the invention features a method of identifying a potential modulator of PTK function as a modulator of PTK function. The method comprises the steps of: (a) administering a potential modulator of PTK function to cells; (b) comparing the level of cell growth between cells not administered the potential modulator and cells administered the potential modulator; and (c) identifying the potential modulator as a modulator of PTK function based on the difference in cell growth.

The term "cell growth" refers to the rate at which a group of cells divides. Cell division rates can be readily measured by methods utilized by those skilled in the art.

Another aspect of the invention features a method of diagnosing a disease by identifying cells harboring a PTK with inappropriate activity. The method comprises the steps of: (a) administering a modulator of PTK function to cells; (b) comparing the rate of cell growth between cells not administered the modulator and cells administered the modulator; and (c) diagnosing a disease by characterizing cells harboring a PTK with inappropriate activity from the effect of the modulator on the difference in the rate of cell growth. The modulator can be identified by the methods of the

invention.

The term "inappropriate activity" refers to a PTK that regulates a step in a signal transduction process at a higher or lower rate than normal cells.

Aberrations in the rate of signal transduction can be caused by alterations in the stimulation of a receptor PTK by a growth factor, alterations in the activity of PTK-specific phosphatase, over-expression of a PTK in a cell, or mutations in the catalytic region of the PTK itself.

The term "signal transduction process" describes the steps in a cascade of events where an extracellular signal is transmitted into an intracellular signal.

The term "PTK-specific phosphatase" describes an enzyme that dephosphorylates a particular PTK and thereby regulates that PTK's activity.

Another aspect of the invention is a method of treating a disease associated with a PTK with inappropriate activity in a cellular organism, where the method comprises the steps of: (a) administering the modulator of PTK function to the organism, where the modulator is in an acceptable pharmaceutical preparation; and (b) activating or inhibiting the PTK function to treat the disease.

The term "organism" relates to any living being comprised of at least one cell. An organism can be as simple as one eukaryotic cell or as complex as a mammal.

The term "administering", in reference to an organism, refers to a method of introducing the compound to the organism. The compound can be administered when the cells or tissues of the organism exist within the

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organism or outside of the organism. Cells existing outside the organism can be maintained or grown in cell culture dishes. For cells harbored within the organism, many techniques exist in the art to administer compounds, including (but not limited to) oral, parenteral, dermal, and injection applications. cells outside of the patient, multiple techniques exist in the art to administer the compounds, including (but not limited to) cell microinjection techniques, transformation techniques, and carrier techniques.

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The term "pharmaceutically acceptable composition" refers to a preparation comprising the modulator of PTK activity. The composition is acceptable if it does not appreciably cause irritations to the organism administered the compound.

Preferred embodiments of the of the invention are that the PTK is a receptor PTK selected from the group consisting of FGF-R, PDGF-R, FLK-1, CCK4, MET, TRKA, AXL, TIE, EPH, RYK, DDR, ROS, RET, LTK, ROR1, and MUSK. Other preferred embodiments of the invention are that the PTK is a non-receptor PTK selected from the group consisting of SRC, BRK, BTK, CSK, ABL, ZAP70, FES, FAK, JAK, and ACK.

The summary of the invention described above is non-limiting and other features and advantages of the invention will be apparent from the following detailed description, and from the claims.

#### BRIEF DESCRIPTION OF THE FIGURES

FIG. 1 provides a ribbon diagram of the structure 30 of FGFR1 showing the side chains of tyrosines Tyr-653

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and Tyr-654 and the  $\alpha$  helical ( $\alpha$ C,  $\alpha$ D,  $\alpha$ E,  $\alpha$ EF,  $\alpha$ F- $\alpha$ I),  $\beta$  strand ( $\beta$ 1- $\beta$ 5,  $\beta$ 7,  $\beta$ 8), nucleotide-binding loop, catalytic loop, activation loop and kinase insert regions of the molecule. The termini are denoted by N and C. The loop between  $\beta$ 2 and  $\beta$ 3 is disordered, indicated by a break in the chain in this region.

FIG. 2 provides a stereo view of a  $C_{\alpha}$  trace of FGFR1 shown in the same orientation as FIG. 1, with every tenth amino acid residue marked with a filled circle and every twentieth amino acid residue labeled with a residue number.

FIG. 3 provides a structure-based sequence alignment of human fibroblast growth factor receptor 1 (FGFR1), human fibroblast growth factor receptor 2 (FGFR2), human fibroblast growth factor receptor 3 (FGFR3), human fibroblast growth factor receptor 4 (FGFR4), a D. malanogaster homolog (DFGFR1), a C. elegans homolog (EGL-15) and insulin receptor tyrosine kinase (IRK).

FIGS. 4A and 4B provide ribbon diagrams of the N-terminal lobes (4A) and C-terminal lobes (4B) of FGFR1 and IRK in which the  $C_{\alpha}$  atoms of the  $\beta$  sheets (4A) or  $\alpha$ -helices (4B) of the two proteins have been superimposed.

FIG. 5 illustrates the side-chain positions of the tyrosine autophosphorylation sites of FGFR1 on the backbone representation of FGFR1.

FIGS. 6A and 6B are amino acid sequence alignments of the catalytic domains of PTKs, including receptor and non-receptor type PTKs. FIG. 6A depicts one

representative member from each of the eighteen subfamilies of receptor tyrosine kinases. FIG. 6B

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depicts one representative member from each of the subfamilies of cytoplasmic tyrosine kinases. In FIGS. 6A and 6B highly conserved residues are boxed. The position of the glycine-rich domain, kinase insert, catalytic loop, and activation loop are indicated. The numbering is for human FGF-receptor.

# BRIEF DESCRIPTION OF THE CRYSTALLOGRAPHIC ATOMIC STRUCTURAL COORDINATES

10 The crystallographic structural coordinates are located at the end of the section entitled "Examples" and before the claims. Three sets of coordinates can be found in the Protein Data Bank under accession names 1FGK, 1AGW, and 1FGI. The 1FGK coordinates correspond to those listed in Table 1, the 1AGW coordinates correspond to those listed in Table 4, and the 1FGI coordinates correspond to those listed in Table 3. The 1AGW and 1FGI coordinate sets will be publically available in March 1998.

Table 1 provides the atomic structure coordinates of native FGFR1 crystals of the invention as determined by X-ray crystallography; and

Table 2 provides the atomic structure coordinates of FGFR1:AMP-PCP co-crystals of the invention as determined by X-ray crystallography.

Table 3 lists crystallographic coordinates defining the three dimensional structure of FGF-R1 complexed with 3-[(3-(2-carboxyethyl)-4-methylpyrrol-5-yl)methylene]-2-indolinone. The columns (from left to right) are descriptions of the atoms by number and type, amino acid and number containing the atom, the x coordinate, y

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coordinate, z coordinate, bond connectivity, and temperature factor. All of these parameters are well defined in the art.

Table 4 is a file of crystallographic coordinates defining the three dimensional structure of FGF-R1 complexed with 3-[4-(4-formylpiperazine-1-yl) benzylidenyl]-2-indolinone. The columns are as described in Table 3.

# DETAILED DESCRIPTION OF THE INVENTION

The present invention is directed to the design and identification of modulators of protein tyrosine kinase function that are PTK subfamily specific, non-hydrolyzable under acidic conditions, and highly bioavailable. The three dimensional structures of a PTK optionally complexed with compounds can facilitate design and identification of modulators of PTK function.

Protein tyrosine kinases (PTKs) comprise a large and diverse class of enzymes. Schlessinger and Ullrich, 1992, Neuron 9: 383-391. The PTK family is subdivided into members that are receptors and those that are non-receptors. The PTK receptor family contains multiple subfamilies, one of which is the fibroblast growth factor receptor (FGF-R) PTK which is a molecule implicated in regulating angiogenesis a well as cellular proliferation and differentiation. Givol and Yayon, 1992, FASEB J. 6 (15): 3362-3369.

FGF-R1 can mediates cellular functions by its role in one or more cellular signal transduction processes. Cellular signal transduction processes comprise multiple steps that convert an extracellular signal into an

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intracellular signal.

Receptor PTK mediated signal transduction is initiated by binding a specific extracellular ligand, followed by receptor dimerization, and subsequent autophosphorylation of the receptor PTK. The phosphate groups are binding sites for intracellular signal transduction molecules which leads to the formation of protein complexes at the cell membrane. These complexes facilitate an appropriate cellular effect (e.g., cell division, metabolic effects to the extracellular microenvironment) in response to the ligand that began the cascade of events.

Receptor PTKs function as binding sites for several intracellular proteins. Intracellular PTK binding 15 proteins are divided into two principal groups: (1) those which harbor a catalytic domain; and (2) those which lack such a domain but serve as adapters and associate with catalytically active molecules. Songyang et al., 1993, Cell 72:767-778. SH2 (src homology) 20 domains are common adaptors found in proteins which directly bind to the receptor PTK. SH2 domains are harbored by PTK binding proteins of both groups mentioned above. Fantl et al., 1992, Cell 69:413-423; Songyang et al., 1994, Mol. Cell. Biol. 14:2777-2785); 25 Songyang et al., 1993, Cell 72:767-778; and Koch et al., 1991, Science 252:668-678.

The specificity of the interactions between receptor PTKs and the SH2 domains of their binding proteins is determined by the amino acid residues immediately surrounding the phosphorylated tyrosine residue. Differences in the binding affinities of SH2

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domains is correlated with the observed differences in substrate phosphorylation profiles of downstream molecules in the signal transduction process. Songyang et al., 1993, Cell 72:767-778. These observations suggest that the function of each receptor PTK is determined not only by its pattern of expression and ligand availability but also by the array of downstream signal transduction pathways that are activated by a particular receptor. Thus, PTKs provide a controlling regulatory role in signal transduction processes as a consequence of autophosphorylation.

PTK-mediated signal transduction regulates cell proliferative, differentiation, and metabolic responses in cells. Therefore, inappropriate PTK activity can result in a wide array of disorders and diseases. These disorders, which are described below, may be treated by the modulators of PTK function designed or identified by the methods disclosed herein.

The present invention also relates to crystalline 20 polypeptides corresponding to the catalytic domain of receptor tyrosine kinases. Such tyrosine kinases include receptors of a class that are not covalently cross-linked but are understood to undergo ligandinduced dimerization, as well as cytoplasmic tyrosine kinases. Preferably, the crystalline catalytic domains 25 are of sufficient quality to allow for the determination of a three-dimensional X-ray diffraction structure to a resolution of about 1.5 Å to about 2.5 Å. The invention also relates to methods for preparing and crystallizing the polypeptides. The polypeptides themselves, as well 30 as information derived from their crystal structures can

be used to analyze and modify tyrosine kinase activity as well as to identify compounds that interact with the catalytic domain.

The polypeptides of the invention are designed on 5 the basis of the structure of a region in the cytoplasmic domain of the receptor tyrosine kinase that contains the catalytic domain. By way of illustration, FIG. 6A shows the amino acid sequence alignment of the catalytic domains of eighteen human receptor tyrosine 10 kinases; one representative member from each of the eighteen subfamilies is shown. FIG. 6B shows the alignment for cytoplasmic kinases. The applicants have discovered and determined the boundaries of the domain required for crystallization of the resulting 15 polypeptide. Surprisingly, these boundaries differ from that required for catalytic activity. For example, referring to FIG. 6A, the domain required for catalytic activity is generally believed to span about 7 amino acid residues upstream of the first glycine (FIG. 6A 20 residue number 485) of the N-terminal glycine-rich region through about 10 residues beyond the C-terminal conserved arginine (FIG. 6A, residue number 744). However, the additional sequence upstream of the Nterminal glycine-rich region and downstream of the C-25 terminal conserved arginine can be required for crystallization. In particular, at least about 20 amino acid residues (+/- 5 amino acid residues) upstream of the first glycine (i.e., FIG. 6A, residue number 485) in the conserved glycine-rich region of the catalytic 30 domain, and at least about 17 amino acid residues (+/- 5 amino acid residues) downstream of the conserved

arginine (<u>i.e.</u>, FIG. 6A, residue number 744) located at the C-terminal boundary of the catalytic domain can be required to engineer a polypeptide suitable for crystallization.

5 In those situations where the resulting polypeptide contains cysteine residues that interfere with crystallization (e.g., cysteine residue numbers 488 and 584 in the FGF-R1 sequence shown in FIG. 6A), such cysteine residues can be substituted with an appropriate 10 amino acid that does not readily form covalent bonds with other amino acid residues under crystallization conditions; e.g., by substituting the cysteine with Ala, Ser or Gly. Any cysteine located in a non-helical or non- $\beta$ -stranded segment, based on secondary structure  $\mathcal{L}$ 15 assignments, are good candidates for replacement. example, cysteines located in regions corresponding to the glycine-rich-loop, the kinase insert, the juxtamembrane region or the activation loop are prime candidates for replacement. However, substitutions of 20 cysteine residues that are conserved among the kinases (e.g., FIG. 6A at positions 725 and 736) are preferably avoided.

#### PTK Associated Diseases

Blood vessel proliferative disorders refer to angiogenic and vasculogenic disorders generally resulting in abnormal proliferation of blood vessels. The formation and spreading of blood vessels play important roles in a variety of physiological processes such as embryonic development, corpus luteum formation, wound healing and organ regeneration. They also play a

pivotal role in cancer development. Other examples of blood vessel proliferation disorders include arthritis, where new capillary blood vessels invade the joint and destroy cartilage, and ocular diseases, like diabetic retinopathy, where new capillaries in the retina invade the vitreous, bleed and cause blindness. Conversely, disorders related to the shrinkage, contraction or closing of blood vessels are implicated in such diseases as restenosis.

10 Fibrotic disorders refer to the abnormal formation of extracellular matrix. Examples of fibrotic disorders include hepatic cirrhosis and mesangial cell proliferative disorders. Hepatic cirrhosis is characterized by the increase in extracellular matrix constituents resulting in the formation of a hepatic scar. Hepatic cirrhosis can cause diseases such as cirrhosis of the liver. An increased extracellular matrix resulting in a hepatic scar can also be caused by viral infection such as hepatitis.

Mesangial cell proliferative disorders refer to disorders brought about by abnormal proliferation of mesangial cells. Mesangial proliferative disorders include various human renal diseases, such as glomerulonephritis, diabetic nephropathy, malignant nephrosclerosis, thrombotic microangiopathy syndromes, transplant rejection, and glomerulopathies. The PDGF-R has been implicated in the maintenance of mesangial cell proliferation. Floege et al., 1993, Kidney International 43:478-548.

PTKs are directly associated with the cell proliferative disorders described above. For example,

some members of the receptor PTK family have been associated with the development of cancer. Some of these receptors, like EGFR (Tuzi et al., 1991, Br. J. Cancer 63:227-233; Torp et al., 1992, APMIS 100:713-

- 719) HER2/neu (Slamon et al., 1992, APMIS 100:713-and PDGF-R (Kumabe et al., 1992, Oncogene 7:627-633) are over-expressed in many tumors and/or persistently activated by autocrine loops. In fact, PTK over-expression (Akbasak and Suner-Akbasak et al., 1992, J.
- Neurol. Sci. 111:119-133; Dickson et al., 1992, J. Treatment Res. 61:249-273; Korc et al., 1992, J. Clin. Invest. 90:1352-1360) and autocrine loop stimulation (Lee and Donoghue, 1992, J. Cell. Biol. 118:1057-1070; Korc et al., supra; Akbasak and Suner-Akbasak et al.,
- supra) account for the most common and severe cancers. For example, EGFR is associated with squamous cell carcinoma, astrocytoma, glioblastoma, head and neck cancer, lung cancer and bladder cancer. HER2 is associated with breast, ovarian, gastric, lung, pancreas
- and bladder cancer. PDGF-R is associated with glioblastoma, lung, ovarian, melanoma and prostate cancer. The receptor PTK c-met is generally associated with hepatocarcinogenesis and thus hepatocellular carcinoma. Additionally, c-met is linked to malignant
- tumor formation. More specifically, c-met has been associated with, among other cancers, colorectal, thyroid, pancreatic and gastric carcinoma, leukemia and lymphoma. Additionally, over-expression of the c-met gene has been detected in patients with Hodgkins
- disease, Burkitts disease, and the lymphoma cell line.

  The IGF-I receptor PTK, in addition to being

implicated in nutritional support and in type-II diabetes, is also associated with several types of cancers. For example, IGF-I has been implicated as an autocrine growth stimulator for several tumor types, 5 e.g. human breast cancer carcinoma cells (Arteaga et al., 1989, J. Clin. Invest. 84:1418-1423) and small lung tumor cells (Macauley et al., 1990, Cancer Res. 50:2511-2517). In addition, IGF-I, integrally involved in the normal growth and differentiation of the nervous system, 10 appears to be an autocrine stimulator of human gliomas. Sandberg-Nordqvist et al., 1993, Cancer Res. 53:2475-The importance of the IGF-IR and its modulators in cell proliferation is further supported by the fact that many cell types in culture (fibroblasts, epithelial 15 cells, smooth muscle cells, T-lymphocytes, myeloid cells, chondrocytes, osteoblasts, the stem cells of the bone marrow) are stimulated to grow by IGF-I. Goldring and Goldring, 1991, Eukaryotic Gene Expression 1:301-In a series of recent publications suggest that 20 IGF-IR plays a central role in the mechanisms of transformation and, as such, could be a preferred target for therapeutic interventions for a broad spectrum of human malignancies. Baserga, 1995, Cancer Res. 55:249-252; Baserga, 1994, Cell 79:927-930; Coppola et al., 25 1994, Mol. Cell. Biol. 14:4588-4595.

The association between abnormalities in receptor PTKs and disease are not restricted to cancer, however. For example, receptor PTKs are associated with metabolic diseases like psoriasis, diabetes mellitus, wound healing, inflammation, and neurodegenerative diseases. EGF-R is indicated in corneal and dermal wound healing.

Defects in Insulin-R and IGF-IR are indicated in type-II diabetes mellitus. A more complete correlation between specific receptor PTKs and their therapeutic indications is set forth in Plowman et al., 1994, DN&P 7:334-339.

Non-receptor PTKs, including src, abl, fps, yes, fyn, lyn, lck, blk, hck, fgr, yrk (reviewed by Bolen et al., 1992, FASEB J. 6:3403-3409), are involved in the proliferative and metabolic signal transduction pathways also associated with receptor PTKs. Therefore, the present invention is also directed towards designing modulators against this class of PTKs. For example, mutated src (v-src) is an oncoprotein (pp60v-src) in

chicken. Moreover, its cellular homolog, the protooncogene pp60<sup>c-src</sup> transmits oncogenic signals of many
receptors. For example, over-expression of EGF-R or
HER2/neu in tumors leads to the constitutive activation
of pp60<sup>c-src</sup>, which is characteristic of the malignant
cell but absent in the normal cell. On the other hand,

osteopetrotic phenotype, indicating a key participation of c-src in osteoclast function and a possible involvement in related disorders. Similarly, Zap 70 is implicated in T-cell signaling. Both receptor PTKs and non-receptor PTKs are connected to hyperimmune

The instant invention is directed in part towards designing modulators of PTK function that could indirectly kill tumors by cutting off their source of sustenance. Normal vasculogenesis and angiogenesis play important roles in a variety of physiological processes such as embryonic development, wound healing, organ

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regeneration and female reproductive processes such as follicle development in the corpus luteum during ovulation and placental growth after pregnancy. Folkman and Shing, 1992, J. Biological Chem. 267:10931-34. However, many diseases are driven by persistent unregulated or inappropriate angiogenesis. For example, in arthritis, new capillary blood vessels invade the joint and destroy the cartilage. In diabetes, new capillaries in the retina invade the vitreous, bleed and cause blindness. Folkman, 1987, in: Congress of Thrombosis and Haemostasis (Verstraete, et. al, eds.), Leuven University Press, Leuven, pp.583-596. Ocular neovascularization is the most common cause of blindness

Moreover, vasculogenesis and/or angiogenesis can be associated with the growth of malignant solid tumors and metastasis. A tumor must continuously stimulate the growth of new capillary blood vessels for the tumor itself to grow. Furthermore, the new blood vessels embedded in a tumor provide a gateway for tumor cells to enter the circulation and to metastasize to distant sites in the body. Folkman, 1990, J. Natl. Cancer Inst. 82:4-6; Klagsbrunn and Soker, 1993, Current Biology 3:699-702; Folkman, 1991, J. Natl., Cancer Inst. 82:4-6; Weidner et al., 1991, New Engl. J. Med. 324:1-5.

and dominates approximately twenty (20) eye diseases.

Several polypeptides with in vitro endothelial cell growth promoting activity have been identified. Examples include acidic and basic fibroblastic growth factor ( $\alpha$ FGF,  $\beta$ FGF), vascular endothelial growth factor (VEGF) and placental growth factor. Unlike  $\alpha$ FGF and  $\beta$ FGF, VEGF has recently been reported to be an

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endothelial cell specific mitogen. Ferrara and Henzel, 1989, Biochem. Biophys. Res. Comm. 161:851-858; Vaisman et al., 1990, J. Biol. Chem. 265:19461-19566.

Thus, identifying the specific receptors that bind FGF or VEGF is important for understanding endothelial 5 cell proliferation regulation. Two structurally related receptor PTKs that bind VEGF with high affinity are identified: the flt-1 receptor (Shibuya et al., 1990, Oncogene 5:519-524; De Vries et al., 1992, Science

- 255:989-991) and the KDR/FLK-1 receptor, discussed in 10 the U.S. Patent Application No. 08/193,829. addition, a receptor that binds  $\alpha FGF$  and  $\beta FGF$  is identified. Jaye et al., 1992, Biochem. Biophys. Acta 1135:185-199). Consequently, these receptor PTKs most 15
- likely regulate endothelial cell proliferation. FGFRs play important roles in angiogenesis, wound healing, embryonic development, and malignant transformation. Basilico and Moscatelli, 1992, Adv.

Cancer Res. 59:115-165. Four mammalian FGFR (FGFR1-4)

- have been described and additional diversity is 20 generated by alternative RNA splicing within the extracellular domains. Jaye et al., 1992, Biochem. Biophys. Acta 1135:185-199. Like other receptor PTKs, dimerization of FGF receptors is essential for their
- 25 activation. Soluble or cell surface-bound heparin sulfate proteoglycans act in concert with FGF to induce dimerization (Schlessinger et al., 1995, Cell 83:357-360), which leads to autophosphorylation of specific tyrosine residues in the cytoplasmic domain. Mohammadi 30
- et al., 1996, Mol. Cell Biol. 16:977-989.

Mutations in three human FGF receptor genes, FGFR1,



FGFR2, and FGFR3, have been implicated in a variety of human genetic skeletal disorders. Mutations in FGFR1 and FGFR2 result in the premature fusion of the flat bones of the skull and cause the craniosynostosis syndromes, such as Apert (FGFR2) (Wilkie et al., 1994, 5 Nat. Genet. 8:269-274), Pfeiffer (FGFR1 and FGFR2) (Muenke et al., 1994, Nat. Genet. 8:269-274), Jackson-Weiss (FGFR2) (Jabs et al., 1994, Nat. Genet. 8:275-279) and Crouzon (FGFR2) (Jabs et al., 1994, Nat. 10 Genet. 8:275-279) syndromes. In contrast mutations in FGFR3 are implicated in long bone disorders and cause several clinically related forms of dwarfism including achondroplasia (Shiang et al., 1994, Cell 78:335-342), hypochondroplasia (Bellus et al., 1995, Nat. Genet. 15 10:357-359) and the neonatal lethal thanatophoric dysplasia (Tavormina et al., 1995, Nat. Genet. 9:321-328). It has been shown that these mutations lead to constitutive activation of the tyrosine kinase activity of FGFR3 (Webster et al., 1996, EMBO J. 15:520-527). 20 Furthermore gene-targeting experiments in mice have revealed an essential role for FGFR3 in developmental bone formation (Deng et al., 1996, Cell 84:911-921). Another major role proposed for FGFs in vivo is the induction of angiogenesis (Folkman and Klagsbrun, 1987, 25 Science 236:442). Therefore, inappropriate expression of FGFs or of their receptors or aberrant function of the tyrosine kinase activity could contribute to several human angiogenic pathologies such as diabetic retinopathy, rheumatoid arthritis, atherosclerosis and

tumor neovascularization (Klagsbrun and Edelman, 1989,

Arteriosclerosis 9:269). Moreover, FGFs are thought to

be involved in malignant transformation. genes coding for the three FGF homologues int-2, FGF-5 and hst-1/K-fgf were originally isolated as oncogenes. Furthermore, the cDNA encoding FGFR1 and FGFR2 are

- amplified in a population of breast cancers (Adnane et 5 al., 1991, Oncogene 6:659-663). Over-expression of FGF receptors has been also detected in human pancreatic cancers, astrocytomas, salivary gland adenosarcomas, Kaposi sarcomas, ovarian cancers and prostate cancers.
- 10 Evidence, such as the disclosure set forth in copending U.S. Application Serial No. 08/193,829, strongly suggests that VEGF is not only responsible for endothelial cell proliferation, but also is a prime regulator of normal and pathological angiogenesis. See
- generally, Klagsburn and Soker, 1993, Current Biology 15 3:699-702; Houck et al., 1992, J. Biol. Chem. 267:26031-26037. Moreover, it has been shown that KDR/FLK-1 and flt-1 are abundantly expressed in the proliferating endothelial cells of a growing tumor, but 20
- not in the surrounding quiescent endothelial cells. Plate et al., 1992, Nature 359:845-848; Shweiki et al., 1992, Nature 359:843-845.

The invention is directed to designing and identifying modulators of receptor and non-receptor PTKfunctions that could modify the inappropriate activity 25 of a PTK involved with a clinical disorder. rational design and identification of modulators of PTKfunctions can be accomplished by utilizing the structural coordinates that define a PTK three dimensional structure.

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## II. <u>Modulators of PTK functions as Therapeutics for</u> Disease

As a consequence of the disorders discussed above, scientists in the biomedical community are searching for modulators of PTK functions that down-regulate signal transduction pathways associated with inappropriate PTK activity.

In particular, small molecule modulators of PTK functions are sought as some can traverse the cell 10 membrane and do not hydrolyze in acidic environments. Some compounds have already been discovered. example, bis monocyclic, bicyclic or heterocyclic aryl compounds (PCT WO 92/20642), vinylene-azaindole derivatives (PCT WO 94/14808) 1-cyclopropyl-4-pyridyl-15 quinolones (U.S. Patent No. 5,330,992), styryl compounds (U.S. Patent No. 5,217,999), styryl-substituted pyridyl compounds (U.S. Patent No. 5,302,606), certain quinazoline derivatives (EP Application No. 0 566 266 Al), seleoindoles and selenides (PCT WO 94/03427), 20 tricyclic polyhydroxylic compounds (PCT WO 92/21660), and benzylphosphonic acid compounds (PCT WO 91/15495) are described as PTK inhibitors.

Although some modulators of PTK function are known, many of these are not specific for PTK subfamilies and will therefore cause multiple side-effects as therapeutics. Compounds of the oxindolinone/ thiolindolinone family, however, are specific for the FGF receptor subfamily (U.S. Patent Application Serial No. 08/702,232, filed August 23, 1996, invented by Tang et al., entitled "Indolinone Combinatorial Libraries and Related Products and Methods for the Treatment of

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Disease," Attorney Docket No. 221/187). In addition, compounds of the oxindolinone/thiolindolinone family are non-hydrolyzable in acidic conditions and can be highly bioavailable.

5 The invention provides information regarding the specific interactions between a PTK and compounds of the oxindolinone/thiolindolinone family. Although the use of X-ray crystallography has provided three dimensional structures of other PTKs, the PTKs in these structures 10 are not complexed with PTK subfamily specific, hydrolysis resistant, highly bioavailable small molecules. The X-ray crystallography techniques used in the current invention resolve interactions between a PTK and compounds in complex with it at the atomic level, which provides detailed information regarding the 15 orientation of chemical groups defining an effective modulator of PTK function.

## III. Crystalline Tyrosine Kinases

Crystalline PTKs of the invention include native crystals, derivative crystals and co-crystals. The native crystals of the invention generally comprise substantially pure polypeptides corresponding to the tyrosine kinase domain in crystalline form.

It is to be understood that the crystalline tyrosine kinase domains of the invention are not limited to naturally occurring or native tyrosine kinase domains. Indeed, the crystals of the invention include mutants of native tyrosine kinase domains. Mutants of native tyrosine kinase domains are obtained by replacing at least one amino acid residue in a native tyrosine

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kinase domain with a different amino acid residue, or by adding or deleting amino acid residues within the native polypeptide or at the N- or C-terminus of the native polypeptide, and have substantially the same three-dimensional structure as the native tyrosine kinase domain from which the mutant is derived.

By having substantially the same three-dimensional structure is meant having a set of atomic structure coordinates that have a root-mean-square deviation of less than or equal to about  $2\dot{A}$  when superimposed with the atomic structure coordinates of the native tyrosine kinase domain from which the mutant is derived when at least about 50% to 100% of the  $C\alpha$  atoms of the native tyrosine kinase domain are included in the superposition.

Amino acid substitutions, deletions and additions which do not significantly interfere with the three-dimensional structure of the tyrosine kinase domain will depend, in part, on the region of the tyrosine kinase domain where the substitution, addition or deletion occurs. In highly variable regions of the molecule, such as those shown in FIG. 6, non-conservative substitutions as well as conservative substitutions may be tolerated without significantly disrupting the three-dimensional structure of the molecule. In highly conserved regions, or regions containing significant secondary structure, such as those regions shown in FIG. 6, conservative amino acid substitutions are preferred.

Conservative amino acid substitutions are wellknown in the art, and include substitutions made on the basis of similarity in polarity, charge, solubility,

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hydrophobicity, hydrophilicity and/or the amphipathic nature of the amino acid residues involved. For example, negatively charged amino acids include aspartic acid and glutamic acid; positively charged amino acids include lysine and arginine; amino acids with uncharged polar head groups having similar hydrophilicity values include the following: leucine, isoleucine, valine; glycine, alanine; asparagine, glutamine; serine, threonine; phenylalanine, tyrosine. Other conservative amino acid substitutions are well known in the art.

For tyrosine kinase domains obtained in whole or in part by chemical synthesis, the selection of amino acids available for substitution or addition is not limited to the genetically encoded amino acids. Indeed, the mutants described herein may contain non-genetically encoded amino acids. Conservative amino acid substitutions for many of the commonly known non-genetically encoded amino acids are well known in the art. Conservative substitutions for other amino acids can be determined based on their physical properties as compared to the properties of the genetically encoded amino acids.

In some instances, it may be particularly advantageous or convenient to substitute, delete and/or add amino acid residues to a native tyrosine kinase domain in order to provide convenient cloning sites in cDNA encoding the polypeptide, to aid in purification of the polypeptide, and for crystallization of the polypeptide. Such substitutions, deletions and/or additions which do not substantially alter the three dimensional structure of the native tyrosine kinase

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domain will be apparent to those of ordinary skill in the art.

It should be noted that the mutants contemplated herein need not exhibit PTK activity. Indeed, amino acid substitutions, additions or deletions that interfere with the kinase activity of the tyrosine kinase domain but which do not significantly alter the three-dimensional structure of the domain are specifically contemplated by the invention. Such crystalline polypeptides, or the atomic structure coordinates obtained therefrom, can be used to identify compounds that bind to the native domain. These compounds may affect the activity or the native domain.

The derivative crystals of the invention generally comprise a crystalline tyrosine kinase domain polypeptide in covalent association with one or more heavy metal atoms. The polypeptide may correspond to a native or a mutated tyrosine kinase domain. Heavy metal atoms useful for providing derivative crystals include, by way of example and not limitation, gold, mercury, etc.

The co-crystals of the invention generally comprise a crystalline tyrosine kinase domain polypeptide in association with one or more compounds. The association may be covalent or non-covalent. Such compounds include, but are not limited to, cofactors, substrates, substrate analogues, inhibitors, allosteric effectors, etc.

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IV. Three Dimensional Structure Determination Using Xray Crystallography

X-ray crystallography is a method of solving the three dimensional structures of molecules. The structure of a molecule is calculated from X-ray diffraction patterns using a crystal as a diffraction grating. Three dimensional structures of protein molecules arise from crystals grown from a concentrated aqueous solution of that protein. The process of X-ray crystallography can include the following steps:

- (a) synthesizing and isolating a polypeptide;
- (b) growing a crystal from an aqueous solution comprising the polypeptide with or without a modulator; and
- (c) collecting X-ray diffraction patterns from the crystals, determining unit cell dimensions and symmetry, determining electron density, fitting the amino acid sequence of the polypeptide to the electron density, and refining the structure

## Production of Polypeptides

The native and mutated tyrosine kinase domain

polypeptides described herein may be chemically
synthesized in whole or part using techniques that are
well-known in the art (see, e.g., Creighton, 1983).

Alternatively, methods which are well known to those
skilled in the art can be used to construct expression
vectors containing the native or mutated tyrosine kinase
domain polypeptide coding sequence and appropriate

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transcriptional/translational control signals. These methods include in vitro recombinant DNA techniques, synthetic techniques and in vivo recombination/genetic recombination. See, for example, the techniques described in Maniatis et al., 1989 and Ausubel et al., 1989.

A variety of host-expression vector systems may be utilized to express the tyrosine kinase domain coding sequence. These include but are not limited to microorganisms such as bacteria transformed with recombinant bacteriophage DNA, plasmid DNA or cosmid DNA expression vectors containing the tyrosine kinase domain coding sequence; yeast transformed with recombinant yeast expression vectors containing the tyrosine kinase domain coding sequence; insect cell systems infected with recombinant virus expression vectors (e.g., baculovirus) containing the tyrosine kinase domain coding sequence; plant cell systems infected with recombinant virus expression vectors (e.g., cauliflower mosaic virus, CaMV; tobacco mosaic virus; TMV) or transformed with recombinant plasmid expression vectors (e.g., Ti plasmid) containing the tyrosine kinase domain coding sequence; or animal cell systems. The expression elements of these systems vary in their strength and specificities.

Depending on the host/vector system utilized, any of a number of suitable transcription and translation elements, including constitutive and inducible promoters, may be used in the expression vector. For example, when cloning in bacterial systems, inducible promoters such as pL of bacteriophage  $\lambda$ , plac, ptrp,

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marker.

ptac (ptrp-lac hybrid promoter) and the like may be used; when cloning in insect cell systems, promoters such as the baculovirus polyhedrin promoter may be used; when cloning in plant cell systems, promoters derived from the genome of plant cells (e.g., heat shock promoters; the promoter for the small subunit of RUBISCO; the promoter for the chlorophyll a/b binding protein) or from plant viruses (e.g., the 35S RNA promoter of CaMV; the coat protein promoter of TMV) may be used; when cloning in mammalian cell systems, promoters derived from the genome of mammalian cells (e.g., metallothionein promoter) or from mammalian viruses (e.g., the adenovirus late promoter; the vaccinia virus 7.5K promoter) may be used; when generating cell lines that contain multiple copies of the tyrosine kinase domain DNA, SV40-, BPV- and EBV-

based vectors may be used with an appropriate selectable

Methods describing methods of DNA manipulation, 20 vectors, various types of cells used, methods of incorporating the vectors into the cells, expression techniques, protein purification and isolation methods, and protein concentration methods are disclosed in detail with respect to the protein PYK-2 in PCT 25 publication WO 96/18738. This publication is incorporated herein by reference in its entirety, including any drawings. Those skilled in the art will appreciate that such descriptions are applicable to the present invention and can be easily adapted to it.

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#### Crystal Growth

Crystals are grown from an aqueous solution containing the purified and concentrated polypeptide by a variety of techniques. These techniques include batch, liquid, bridge, dialysis, vapor diffusion, and hanging drop methods. McPherson, 1982, John Wiley, New York; McPherson, 1990, Eur. J. Biochem. 189:1-23; Webber, 1991, Adv. Protein Chem. 41:1-36, incorporated by reference herein in its entirety, including all figures, tables, and drawings.

Generally, the native crystals of the invention are grown by adding precipitants to the concentrated solution of the polypeptide corresponding to the PTK catalytic domain. The precipitants are added at a concentration just below that necessary to precipitate the protein. Water is removed by controlled evaporation to produce precipitating conditions, which are maintained until crystal growth ceases.

For crystals of the invention, it has been found that hanging drops containing about 2.0  $\mu$ L of tyrosine kinase domain polypeptide (10 mg/mL in 10mM Tris-HCl, pH 8.0, 10 mM NaCl and 2 mM dithiothreitol) and 2.0  $\mu$ L reservoir solution (16% w/v polyethylene glycol MW 10000, 0.3 M (NH<sub>4</sub>)<sub>2</sub>SO<sub>4</sub>, 5% v/v ethylene glycol or glycerol and 100 mM bis-Tris, pH 6.5) suspended over 0.5 mL reservoir buffer for about 3-4 weeks at 4°C provide crystals suitable for high resolution X-ray structure determination.

Those of ordinary skill in the art will recognize
that the above-described crystallization conditions can
be varied. Such variations may be used alone or in

combination, and include polypeptide solutions containing polypeptide concentrations between about 1 mg/mL and about 60 mg/mL, Tris-HCl concentrations between about 10 mM and about 200 mM, dithiothreitol 5 concentrations between about 0 mM and about 20 mM, pH ranges between about 5.5 and about 7.5; and reservoir solutions containing polyethylene glycol concentrations between about 10% and about 30% (w/v), polyethylene glycol molecular weights between about 1000 and about 20,000,  $(NH_4)_2SO_4$  concentrations between about 0.1 M and 10 about 0.5 M, ethylene glycol or glycerol concentrations between about 0% and about 20% (v/v), bis-Tris concentrations between about 10 mM and about 200 mM, pH ranges between about 5.5 and about 7.5 and temperature ranges between about 0°C and about 25°C. Other buffer solutions may be used such as HEPES buffer, so long as the desired pH range is maintained.

Derivative crystals of the invention can be obtained by soaking native crystals in mother liquor containing salts of heavy metal atoms. It has been found that soaking a native crystal in a solution containing about 0.1 mM to about 5 mM thimerosal, 4chloromeruribenzoic acid or  $\mathrm{KAu}\left(\mathrm{CN}\right)_2$  for about 2 hr to about 72 hr provides derivative crystals suitable for use as isomorphous replacements in determining the X-ray crystal structure of the tyrosine kinase domain polypeptide.

Co-crystals of the invention can be obtained by soaking a native crystal in mother liquor containing compound that bind the kinase domain, or described above, or can be obtained by co-crystallizing the kinase

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domain polypeptide in the presence of one or more binding compounds.

For co-crystals of tyrosine kinase domain polypeptide in co-complex with AMP-PCP, it has been found that co-crystallizing the kinase domain polypeptide in the presence of AMP-PCP using the abovedescribed crystallization conditions for obtaining native crystals with a polypeptide solution additionally containing 10 mM AMP-PCP and 20 mM MgCl<sub>2</sub> yields cocrystals suitable for the high resolution structure determination by X-ray crystallography. Of course, those having skill in the art will recognize that the concentrations of AMP-PCP and MgCl<sub>2</sub> in the polypeptide solution can be varied, alone or in combination with the variations described above for native crystals. variations include polypeptide solutions containing AMP-PCP concentrations between 0.1 mM and 50 mM and MqCl, concentrations between 0 mM and 50 mM.

a PTK catalytic domain complexed with a compound can be grown by one of two methods. In the first method, the modulator is added to the aqueous solution containing the polypeptide corresponding to the PTK catalytic domain before the crystal is grown. In the second

method, the modulator is soaked into an already existing crystal of a polypeptide corresponding to a PTK catalytic domain.

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#### Crystalline FGFR

In one illustrative embodiment, the invention provides crystals of FGFR1. The crystals were obtained by the methods provided in the Examples. The FGFR1 crystals, which may be native crystals, derivative crystals or co-crystals, have monoclinic unit cells (i.e., unit cells wherein  $a\neq b\neq c$ ;  $\alpha=\gamma=90^\circ$ ; and  $\beta>90^\circ$ ) and space group symmetry C2. There are two FGFR1 molecules in the asymmetric unit, related by an approximate two-fold axis.

Two forms of crystalline FGFR1 were obtained. In one form (designated "C2-A form"), the unit cell has dimensions of a=208.3 Å, b=57.2 Å, c=65.5 Å and  $\beta$ =107.2°. In another form (designated "C2-B form"), the unit cell has dimensions of a=211.6 Å, b=51.3 Å, c=66.1 Å and  $\beta$ =107.7°.

Three distinct two-fold related FGFR1 dimers are observed in both the C2-A and C2-B forms of the FGFR1 crystal, one non-crystallographically related dimer and two crystallographically related dimers. 20 crystallographically related dimer comprises the two molecules in the asymmetric unit. The residues making up the dimer interface are located in C-terminal lobe. In this dimer, the C-terminal lobes abut with the N-25 terminal lobes distal to one another. The total amount of surface area buried in the surface is about 950  $\mbox{\AA}^2$ . Very few of the interactions in the interface are of a specific nature, e.g., hydrogen-bonding or close packing of hydrophobic residues.

There are two crystallographically-related dimers in the C2 lattice. In the first dimer, the residues

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that constitute the dimer interface are limited to those in the  $\beta$ -sheet of the N-terminal lobe (amino acid residues 477, 479, 498, 506, 508 and 496). The total surface area buried in this interface is about  $670 \text{ Å}^2$ . The interactions are rather specific. Three hydrophobic residues which are partially solvent-exposed in the monomer, Val-479, Ile-498 and Val-508, come together with their two-fold-related residues to form a compact hydrophobic plug. This plug is capped on either side by a salt bridge between Arg-477 and Glu-496. In addition, two main-chain hydrogen-bonds connect the β-sheets of the two monomers at the start of  $\beta$ 3 (amino acid residues 506 and 508). The residues in this dimer interface, or their residue character, are generally conserved in the mammalian FGF receptors, but not in the invertebrate homologues.

The other crystallographically-related dimer buries about 1650 Ų in its interface. In this dimer, the αC helices of the two monomers are nearly parallel and contact each other at their C-terminal ends. Met-534 and Met-537 are in van der Waals contact with their two-fold-related residues. Other hydrophobic contacts involve Pro-466 with Ile-648 and Pro-469 with Ile-676 and Thr-678. In addition, hydrogen bonds (side-chain to main-chain) are made between Arg-470 and Lys-618 and between His-649 and Glu-464, and there are several water molecules that bridge the two monomers through hydrogen bonding.

In the C2-B form of the crystal, the monomers of this second crystallographically-related dimer are shifted slightly with respect to one another (6°

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rotation), indicating that this interface is somewhat fluid.

In both of the crystallographically-related dimers, the N-termini of the two molecules comprising the dimer point in the same direction and are reasonably close to one another.

# Determining Unit Cell Dimensions and the Three Dimensional Structure of a Polypeptide or Polypeptide Complex

Once the crystal is grown, it can be placed in a glass capillary tube and mounted onto a holding device connected to an X-ray generator and an X-ray detection 15 device. Collection of X-ray diffraction patterns are well documented by those in the art. Ducruix and Geige, 1992, IRL Press, Oxford, England, and references cited therein. A beam of X-rays enter the crystal and then diffract from the crystal. An X-ray detection device 20 can be utilized to record the diffraction patterns emanating from the crystal. Although the X-ray detection device on older models of these instruments is a piece of film, modern instruments digitally record Xray diffraction scattering.

Methods for obtaining the three dimensional structure of the crystalline form of a peptide molecule or molecule complex are well known in the art. Ducruix and Geige, 1992, IRL Press, Oxford, England, and references cited therein. The following are steps in the process of determining the three dimensional structure of a molecule or complex from X-ray diffraction data.

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After the X-ray diffraction patterns are collected from the crystal, the unit cell dimensions and orientation in the crystal can be determined. They can be determined from the spacing between the diffraction emissions as well as the patterns made from these emissions. The unit cell dimensions are characterized in three dimensions in units of Angstroms (one  $\rm \AA=10^{-10}$  meters) and by angles at each vertices. The symmetry of the unit cell in the crystals is also characterized at this stage. The symmetry of the unit cell in the crystal simplifies the complexity of the collected data by identifying repeating patterns. Application of the symmetry and dimensions of the unit cell is described below.

15 Each diffraction pattern emission is characterized as a vector and the data collected at this stage of the method determines the amplitude of each vector. phases of the vectors can be determined using multiple techniques. In one method, heavy atoms can be soaked into a crystal, a method called isomorphous replacement, 20 and the phases of the vectors can be determined by using these heavy atoms as reference points in the X-ray analysis. Otwinowski, 1991, Daresbury, United Kingdom, 80-86. The isomorphous replacement method usually 25 requires more than one heavy atom derivative. another method, the amplitudes and phases of vectors from a crystalline polypeptide with an already determined structure can be applied to the amplitudes of the vectors from a crystalline polypeptide of unknown 30 structure and consequently determine the phases of these vectors. This second method is known as molecular

replacement and the protein structure which is used as a reference must have a closely related structure to the protein of interest. Naraza, 1994, Proteins 11:281-296. Thus, the vector information from a PTK of known structure, such as those reported herein, are useful for the molecular replacement analysis of another PTK with unknown structure.

Once the phases of the vectors describing the unit cell of a crystal are determined, the vector amplitudes 10 and phases, unit cell dimensions, and unit cell symmetry can be used as terms in a Fourier transform function. The Fourier transform function calculates the electron density in the unit cell from these measurements. electron density that describes one of the molecules or one of the molecule complexes in the unit cell can be 15 referred to as an electron density map. The amino acid structures of the sequence or the molecular structures of compounds complexed with the crystalline polypeptide may then fit to the electron density using a variety of 20 computer programs. This step of the process is sometimes referred to as model building and can be accomplished by using computer programs such as TOM/FRODO. Jones, 1985, Methods in Enzymology 115:157-

A theoretical electron density map can then be calculated from the amino acid structures fit to the experimentally determined electron density. The theoretical and experimental electron density maps can be compared to one another and the agreement between these two maps can be described by a parameter called an R-factor. A low value for an R-factor describes a high

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degree of overlapping electron density between a theoretical and experimental electron density map.

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The R-factor is then minimized by using computer programs that refine the theoretical electron density A computer program such as X-PLOR can be used for model refinement by those skilled in the art. Brünger, 1992, Nature 355:472-475. Refinement may be achieved in an iterative process. A first step can entail altering the conformation of atoms defined in an electron density map. The conformations of the atoms can be altered by simulating a rise in temperature which will increase the vibrational frequency of the bonds and modify positions of atoms in the structure. At a particular point in the atomic perturbation process, a force field, which typically defines interactions between atoms in terms of allowed bond angles and bond lengths, Van der Waals interactions, hydrogen bonds, ionic interactions, and hydrophobic interactions, can be applied to the system of atoms. Favorable interactions may be described in terms of free energy and the atoms can be moved over many iterations until a free energy minimum is achieved. The refinement process can be iterated until the Rfactor reaches a minimum value.

The three dimensional structure of the molecule or molecule complex is described by atoms that fit the theoretical electron density characterized by a minimum R-value. A file can then be created for the three dimensional structure that defines each atom by coordinates in three dimensions. Examples of such structural coordinate files are defined in Table 1, Table 2, Table 3, and Table 4.

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#### V. Structures of FGFR1

The present invention provides high-resolution three-dimensional structures and atomic structure coordinates of crystalline FGFR1 and crystalline FGFR1:AMP-PCP co-complex as determined by X-ray crystallography. The specific methods used to obtain the structure coordinates are provided in the examples. The atomic structure coordinates of crystalline FGFR1, obtained from the C2-A form of the crystal to 2.0 Å resolution, are listed in Table 3; the coordinates of crystalline FGFR1:AMP-PCP co-complex, obtained from the C2-A form of the crystal to 2.3 Å resolution are listed in Table 4.

15 Those having skill in the art will recognize that atomic structure coordinates as determined by X-ray crystallography are not without error. Thus, it is to be understood that any set of structure coordinates obtained for crystals of FGFR1, whether native crystals, 20 derivative crystals or co-crystals, that have a root mean square deviation ("r.m.s.d.") of less than or equal to about 1.5 Å when superimposed, using backbone atoms (N,  $C_{\alpha}$ , C and O), on the structure coordinates listed in Table 3 or Table 4 are considered to be identical with the structure coordinates listed in the Tables when at 25 least about 50% to 100% of the backbone atoms of FGFR1 are included in the superposition.

Referring now to FIG. 1, the overall structure of FGFR1 is bi-lobate. The N-terminal lobe of FGFR1 spans amino acid residues 456-567 (FIG. 3) and comprises a curled  $\beta$ -sheet of five anti-parallel strands ( $\beta$ 1- $\beta$ 5) and

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one  $\alpha$ -helix ( $\alpha$ C). The C-terminal lobe spans amino acid residues 568-765 (FIG. 3) and comprises two  $\beta$ -strands ( $\beta$ 7,  $\beta$ 8) and seven  $\alpha$ -helices ( $\alpha$ D,  $\alpha$ E,  $\alpha$ EF,  $\alpha$ F- $\alpha$ I). The secondary structure nomenclature follows that used for IRK (Hubbard et al., 1994) which in turn is based on the assignments for cAPK (Knighton et al., 1991). FIG. 2 shows a stereo view of a  $C_{\alpha}$  trace of FGFR1 in the same orientation as FIG. 1.

A structure-based sequence alignment of the tyrosine kinase domains of human fibroblast growth factor receptor 1 (human FGFR1; labelled FGFR1), human fibroblast growth factor receptors 2, 3 and 4 (labelled FGFR2, FGFR3 and FGFR4, respectively), a D. melanogaster homologue (labelled DFDFR1), a C elegans homologue (labelled EGL-15) and insulin receptor kinase (labelled IRK), is shown in FIG. 3. The sequence of FGFR1, which is not shown in FIG. 3 is identical to the sequence of FGFR1 except that FGFR1 has the following amino acid substitutions and additions: Cys-488 → Ala, Cys-584 → Ser, Leu-457 → Val and an additional five N-terminal amino acids (Ser-Ala-Ala-Gly-Thr). The secondary structure assignments for FGFR1 and IRK were obtained using the Kabsch and Sander algorithm (Kabsch and Sander, 1983) as implemented in PROCHECK (Laskowski et al., 1993). In the FGF receptor sequences, a period represents sequence identity to FGFR1. In the IRK sequence, residues that are identical to FGFR1 are highlighted. A hyphen denotes an insertion.

The numbers under the EGL-15 sequence represent the fractional solvent accessibility (FSA2) of the residue in the FGFR1 structure. The FSA ratio is the ratio of

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the solvent-accessible surface area of a residue in a Gly-X-Gly tripeptide compared to that in the FGFR1 structure. A value of 0 represents an FSA between 0.00 and 0.09; 1 represents an FSA between 0.10 and 0.19, etc. The higher the value, the more solvent-exposed the residue. An asterisk or pound sign in the FSA line indicates that the residue (asterisk) or side chain (pound sign) is not included in the atom model due to disorder. The numbers below the FSA line are the FSAs for those residues that form part of a dimer interface.

The amino acid residue numbers for FGFR1, and hence FGFR1, and IRK provided in FIG. 3 are used in the discussion that follows. Significant differences in the N-terminal lobe of FGFR1 as compared to IRK are found in the loops between  $\beta$  strands and in  $\alpha C.$  Residues from the end of  $\beta 1$  through the beginning of  $\beta 2$  (amino acid residues 485-490) form the nucleotide-binding loop, named because of its role in ATP coordination. This residue stretch contains the protein kinase-conserved GXGXXG sequence motif, where X is any amino acid. loop is poorly ordered in one FGFR1 molecule in the asymmetric unit and disordered (i.e., not included in the atomic model) in the other FGFR1 molecule in the asymmetric unit. The loop between  $\beta1$  and  $\beta3$  is disordered in both FGFR1 molecules comprising the asymmetric unit.

Referring now to FIG. 4A, which provides a ribbon diagram of the N-terminal lobes of FGFR1 and IRK in which the  $C_{\alpha}$  atoms of the  $\beta$ -sheets have been superimposed, it can be seen that in FGFR1  $\alpha C$  is longer by one helical turn than in IRK and is oriented such

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that residues Lys-514 and Glu-531, which are conserved in protein kinases, form a salt bridge (represented by a black line). While not intending to be bound by theory, this salt bridge is believed to be important for proper positioning of the conserved lysine side chain, which coordinates two phosphate oxygens of ATP. The salt bridge is observed in the structures of cAPK (Knighton et al., 1991) and mitogen-activated protein kinase (MAPK) (Zhang et al., 1994).

Referring now to FIG. 4B, which provides a ribbon diagram of the C-terminal lobes of FGFR1 and IRK in which the  $C_{\alpha}$  atoms of the  $\alpha$ -helices have been superimposed, a significant difference is found in the C-terminal helix of FGFR1 when compared to IRK; helix  $\alpha$ I of FGFR1 is longer by seven residues (two helical turns) than its counterpart in IRK. The extended length of  $\alpha$ I is presumably important in the biological functioning of FGF receptors, since the tyrosine autophosphorylation site to which an SH2 domain of PLCy binds is six residues C-terminal to this helix.

The structure of FGFR1 displays an open disposition of the N- and C-terminal lobes. Despite having different sets of lattice contacts, the two FGFR1 molecules in the asymmetric unit have only a 2° difference in relative lobe orientation. It appears as though the stearic interaction between residues in  $\alpha$ C (Glu-531 and Met-534) with Phe-642 and Gly-643 of the protein kinase-conserved DFG sequence at the beginning of the activation loop accounts for the open conformation of FGFR1.

The active site of FGFR1 is characterized by at

least amino acid residues spanning the catalytic loop, activation loop and nucleotide binding loop. Unlike the structure of IRK, in which Tyr-1162 occupies the active site of the molecule, the active sites of both FGFR1 molecules in the asymmetric unit are unoccupied.

The activation loop, which regulates phosphorylation, is characterized by at least resides 640 to 663. Quite surprisingly, while the activation loops of FGFR1 and IRK contain the same number of amino 10 acid residues and share greater than 50% sequence homology, the paths of the polypeptide chains are strikingly dissimilar, diverging at Ala-640 (Gly-1149 in IRK) and reconverging at Val-664 (Val-1173 in IRK). Tyr-653 and Tyr 564 are not bound in the active site. Instead, these residues point away from it. Tyr-653 is 15 in van der Waals contact with several hydrophobic residues (Val-664, Leu-672 and Phe-710) and is hydrogenbonded via its hydroxyl group to a backbone carbonyl oxygen (Leu-672). Tyr-654 is more solvent exposed than 20 Tyr-653, and its only van der Waals contact is with Val-Temperature factor data suggest that the activation loop is relatively mobile and adopts multiple conformations.

The catalytic loop of protein kinases lies between secondary structure elements αE and β7 and contains an invariant aspartic acid residue (Asp-623 in FGFR1) which serves as the catalytic base in the phosphotransfer reaction, abstracting the proton from the hydroxyl group of the substrate tyrosine, serine or threonine. The catalytic loop sequence of FGFR1 comprises at least residues His-621 to Asn-628 (amino acid sequence

HRDLAARN), and is identical to that for IRK and most receptor and non-receptor PTKs.

In addition to the two tyrosine autophosphorylation sites in the activation loop (Tyr-653 and Tyr-654),

there are four other autophosphorylation sites present in the FGFR1 crystals of the invention: one in the juxtamembrane region (Tyr-463), two in the kinase insert (Tyr-583 and Tyr-585) and one in the C-terminal lobe (Tyr-730) (Mohammadi et al., 1996). They exhibit varying degrees of conservation in mammalian FGF receptors: Tyr-463 and Tyr-585 in FGFR1 and 2; Tyr-583 in FGFR1, 2 and 3; and Tyr-730 in FGFR 1, 2, 3 and 4 (FIG. 3).

Referring now to FIG. 5, the positions of the autophosphorylation sites are mapped onto the FGFR1 structure. The juxtamembrane site (Tyr-463) and the residues N-terminal to it are disordered in one of the FGFR1 molecules in the asymmetric unit. In the other molecule in the asymmetric unit Tyr-463 is involved in a lattice contact.

The kinase insert region (the region between helices  $\alpha D$  and  $\alpha E$ ) contains autophosphorylation sites Tyr-583 and Tyr-585 and is disordered in both FGFR1 molecules in the asymmetric unit of the C2-A form of the crystal. In the C2-B form, several lattice contacts partially pin down this region in one of the two FGFR1 molecules in the asymmetric unit, allowing a trace of the polypeptide chain to be made. There is no well-defined secondary structure for these residues. Tyr-730, situated in  $\alpha H$  in the C-terminal lobe, is nearly buried and the side-chain hydroxyl group makes two

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hydrogen-bonds. The side chains of neighboring Met-732 and Met-733 are both buried. Therefore, phosphorylation of Tyr-730 would presumably require prior unfolding of  $\alpha_{\rm H}$ .

Aside from Tyr-730, the five other
autophosphorylation sites (including Tyr-653 and Tyr654) are found in relatively mobile segments of the
FGFR1 molecule. While not intending to be bound by
theory, the spatial positions of the autophosphorylation
sites relative to the active site suggest that
autophosphorylation occurs by a trans mechanism between
two kinase domains, supporting the hypothesis that
ligand-induced receptor dimerization is critical for the
initiation of autophosphorylation events.

The structure of crystalline FGFR1:AMP-PCP cocomplex is essentially similar to that observed for
crystalline FGFR1. There are no significant changes in
the structure of FGFR1 induced by AMP-PCP binding. In
particular, binding of AMP-PCP, and by extension ATP,
does not by itself promote lobe closure under the
crystallization conditions used. Furthermore,
complexation did not result in any noticeable changes in
the conformations of the activation and nucleotidebinding loops.

The crystalline FGFR1:AMP-PCP co-complex contains hydrogen bonds that are present between N1 of adenine and the amide nitrogen of Ala-564 and between N6 of adenine and the carbonyl oxygen of Glu-562. The adenine ring is flanked on one side by Leu-484 and Val-492 (N-terminal lobe) and on the other side by Leu-630 (C-terminal lobe). The ribose hydroxyl groups make no

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direct hydrogen bonds with protein atoms. Lys-514 is hydrogen-bonded to oxygens of the  $\beta$ - and  $\gamma$ -phosphates. There is no unambiguous electron density that would indicate the positions of Mg² ions. Generally, AMP-PCP appears to be coordinated rather loosely to unphosphorylated FGFR1, being bound to the "roof" of the cleft rather than being tightly sandwiched between the two kinase lobes.

#### 10 Structural Differences Between FGF-R and IRK

Several features distinguish the FGF-receptor structure from that of the insulin-receptor tyrosine kinase. These distinctions are likely to be important in signaling by FGF-receptors, and other monomeric receptors that are believed to undergo ligand-induced dimerization.

The most significant difference between the structures of FGFR1 and IRK is the conformation of the activation loop. In FGFR1, the activation loop is disposed such that the binding site for substrate peptides is blocked not by an activation loop tyrosine, as in IRK, but by Arg-661 and PTK-invariant Pro-663, while the ATP binding site is accessible. This represents another molecular mechanism by which a receptor PTK may be autoinhibited. The observed autoinhibition in FGFR1 would appear to be weaker than that in IRK because of fewer specific interactions made by residues in the FGFR1 activation loop (manifested in the relatively higher B-values) and the accessibility of the ATP site. One obvious distinction between the insulin and FGF receptor families is that in the former,

receptors are covalently linked heterotetramers  $(\alpha_2\beta_2)$ , whereas in the latter, receptor dimerization is ligand dependent. Receptors whose kinase domains are always in close proximity may require a stronger autoinhibition mechanism than those receptors that associate only upon ligand binding (Taylor et al., 1995). Since most growth factor receptors undergo ligand-dependent dimerization and activation, the FGF receptor autoinhibition mechanism appears to be a more general one.

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### VI. <u>Uses of the Crystals and Atomic Structure</u> <u>Coordinates</u>

The crystals of the invention, and particularly the atomic structure coordinates obtained therefrom, have a wide variety of uses. For example, the crystals 15 described herein can be used as a starting material in any of the art-known methods of use for receptor and non-receptor tyrosine kinases. Such methods of use include, for example, identifying molecules that bind to the native or mutated catalytic domain of tyrosine 20 The crystals and structure coordinates are particularly useful for identifying compounds that inhibit receptor and non-receptor tyrosine kinases as an approach towards developing new therapeutic agents (see, 25 e.g., Levitzki and Gazit, 1995).

The structure coordinates described herein can be used as phasing models for determining the crystal structures of additional native or mutated tyrosine kinase domains, as well as the structures of co-crystals of such domains with ligands such as inhibitors, agonists, antagonists, and other molecules. The

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structure coordinates, as well as models of the three-dimensional structures obtained therefrom, can also be used to aid the elucidation of solution-based structures of native or mutated tyrosine kinase domains, such as those obtained via NMR. Thus, the crystals and atomic structure coordinates of the invention provide a convenient means for elucidating the structures and functions of receptor and non-receptor tyrosine kinases.

For purposes of clarity and discussion, the crystals of the invention will be described by reference to specific FGFR1 exemplary crystals. Those skilled in the art will appreciate that the principles described herein are generally applicable to crystals of the tyrosine kinase domain of any cytoplasmic tyrosine kinase that undergoes ligand-induced dimerization or receptor tyrosine kinase, including but not limited to the tyrosine kinases of FIG. 6.

VII. Structure Determination for PTKs with Unknown Structure Using Structural Coordinates

Structural coordinates, such as those set forth in Table 1, Table 2, Table 3, and Table 4, can be used to determine the three dimensional structures of PTKs with unknown structure. The methods described below can apply structural coordinates of a polypeptide with known structure to another data set, such as an amino acid sequence, X-ray crystallographic diffraction data, or nuclear magnetic resonance (NMR) data. Preferred embodiments of the invention relate to determining the three dimensional structures of PTKs and related polypeptides. These include receptor PTKs such as FGF-

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R, PDGF-R, KDR, CCK4, MET, TRKA, AXL, TIE, EPH, RYK, DDR, ROS, RET, LTK, ROR1, and MUSK. Non-receptor PTKs such as SRC, BRK, BTK, CSK, ABL, ZAP70, FES, FAK, JAK, and ACK can also be used in the methods described herein.

### Structures Using Amino Acid Homology

Homology modeling is a method of applying structural coordinates of a polypeptide of known structure to the amino acid sequence of a polypeptide of 10 unknown structure. This method is accomplished using a computer representation of the three dimensional structure of a polypeptide or polypeptide complex, the computer representation of amino acid sequences of the polypeptides with known and unknown structures, and 15 standard computer representations of the structures of amino acids. Homology modeling comprises the steps of (a) aligning the amino acid sequences of the polypeptides with and without known structure; (b) 20 transferring the coordinates of the conserved amino acids in the known structure to the corresponding amino acids of the polypeptide of unknown structure; refining the subsequent three dimensional structure; and (d) constructing structures of the rest of the polypeptide. One skilled in the art recognizes that conserved amino 25 acids between two proteins can be determined from the sequence alignment step in step (a).

The above method is well known to those skilled in the art. Greer, 1985, Science 228, 1055. Blundell et al., 1988, Eur. J. Biochem. 172, 513. A computer program currently utilized for homology modeling by

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those skilled in the art is the Homology module in the Insight II modeling package distributed by Molecular Simulations Inc.

Alignment of the amino acid sequence is accomplished by first placing the computer representation of the amino acid sequence of a polypeptide with known structure above the amino acid sequence of the polypeptide of unknown structure. Amino acids in the sequences are then compared and groups of amino acids that are homologous (e.g., amino acid side chains that are similar in chemical nature - aliphatic, aromatic, polar, or charged) are grouped together. This method will detect conserved regions of the polypeptides and account for amino acid insertions or deletions.

Once the amino acid sequences of the polypeptides with known and unknown structures are aligned, the structures of the conserved amino acids in the computer representation of the polypeptide with known structure are transferred to the corresponding amino acids of the polypeptide whose structure is unknown. For example, a tyrosine in the amino acid sequence of known structure may be replaced by a phenylalanine, the corresponding homologous amino acid in the amino acid sequence of unknown structure.

The structures of amino acids located in non-conserved regions are to be assigned manually by either using standard peptide geometries or molecular simulation techniques, such as molecular dynamics. The final step in the process is accomplished by refining the entire structure using molecular dynamics and/or energy minimization.

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The homology modeling method is well known to those skilled in the art and has been practiced using different protein molecules. The three dimensional structure of the polypeptide corresponding to the catalytic domain of a serine/threonine protein kinase, myosin light chain protein kinase, was homology modeled from the cAMP-dependent protein kinase catalytic subunit. Knighton et al., 1992, Science 258:130-135.

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#### 10 Structures Using Molecular Replacement

Molecular replacement is a method of applying the X-ray diffraction data of a polypeptide of known structure to the X-ray diffraction data of a polypeptide of unknown sequence. This method can be utilized to define the phases describing the X-ray diffraction data of a polypeptide of unknown structure when only the amplitudes are known. X-PLOR is a commonly utilized computer software package used for molecular replacement. Brünger, 1992, Nature 355:472-475. is another program used for molecular replacement. Navaza, 1994, Acta Crystallogr. A50:157-163. Preferably, the resulting structure does not exhibit a root-mean-square deviation of more than 3 Å.

A goal of molecular replacement is to align the 25 positions of atoms in the unit cell by matching electron diffraction data from two crystals. A program such as X-PLOR can involve four steps. A first step can be to determine the number of molecules in the unit cell and define the angles between them. A second step can 30 involve rotating the diffraction data to define the orientation of the molecules in the unit cell. A third

step can be to translate the electron density in three dimensions to correctly position the molecules in the unit cell. Once the amplitudes and phases of the X-ray diffraction data is determined, an R-factor can be calculated by comparing electron diffraction maps calculated experimentally from the reference data set and calculated from the new data set. An R-factor between 30-50% indicates that the orientations of the atoms in the unit cell are reasonably determined by this method. A fourth step in the process can be to decrease the R-factor to roughly 20% by refining the new electron density map using iterative refinement techniques described herein and known to those or ordinary skill in the art.

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#### Structures Using NMR Data

Structural coordinates of a polypeptide or polypeptide complex derived from X-ray crystallographic techniques can be applied towards the elucidation of three dimensional structures of polypeptides from nuclear magnetic resonance (NMR) data. This method is used by those skilled in the art. Wuthrich, 1986, John Wiley and Sons, New York: 176-199; Pflugrath et al., 1986, J. Molecular Biology 189:383-386; Kline et al., 1986, J. Molecular Biology 189:377-382. While the secondary structure of a polypeptide is often readily determined by utilizing two-dimensional NMR data, the spatial connections between individual pieces of secondary structure are not as readily determinable. The coordinates defining a three-dimensional structure of a polypeptide derived from X-ray crystallographic

techniques can guide the NMR spectroscopist to an understanding of these spatial interactions between secondary structural elements in a polypeptide of related structure.

5 The knowledge of spatial interactions between secondary structural elements can greatly simplify Nuclear Overhauser Effect (NOE) data from twodimensional NMR experiments. Additionally, applying the crystallographic coordinates after the determination of 10 secondary structure by NMR techniques only simplifies the assignment of NOEs relating to particular amino acids in the polypeptide sequence and does not greatly bias the NMR analysis of polypeptide structure. Conversely, using the crystallographic coordinates to simplify NOE data while determining secondary structure of the polypeptide would bias the NMR analysis of protein structure.

As the analysis of polypeptide structure by NMR methods is a relatively new technique, the use of structural coordinates defining a PTK structure will most likely be utilized more frequently in the near future. As the method progresses, the three dimensional structure analysis of polypeptides of the same size as a PTK catalytic domain will become more frequent.

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VIII. Structure-Based Design of Modulators of PTK Function Utilizing Structural Coordinates Structure-based modulator design and identification methods are powerful techniques that can involve searches of computer data bases containing a wide variety of potential modulators and chemical functional

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groups. The computerized design and identification of modulators is useful as the computer data bases contain more compounds than the chemical libraries, often by an order of magnitude. For reviews of structure-based drug design and identification see Kuntz et al., 1994, Acc. Chem. Res. 27:117; Guida, 1994, Current Opinion in Struc. Biol. 4: 777; Colman, 1994, Current Opinion in Struc. Biol. 4: 868.

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The three dimensional structure of a polypeptide defined by structural coordinates can be utilized by these design methods. The structural coordinates of Table 1, Table 2, Table 3, and Table 4 can be utilized by this method. In addition, the three dimensional structures of receptor and non-receptor PTKs determined by the homology, molecular replacement, and NMR techniques described herein can also be applied to modulator design and identification methods. Thus, the structures of receptor PTKs, FGF-R, PDGF-R, FLK, CCK4, MET, TRKA, AXL, TIE, EPH, RYK, DDR, ROS, RET, LTK, ROR1, and MUSK, can be utilized by the methods described herein. The structures of non-receptor PTKs, SRC, BRK, BTK, CSK, ABL, ZAP70, FES, FAK, JAK, and ACK, can also be utilized by the rational modulator design method.

#### 25 <u>Design by Searching Molecular Data Bases</u>

One method of rational modulator design searches for modulators by docking the computer representation of compounds from a data base of molecules. Publicly available data bases include:

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a) ACD from Molecular Designs Limited

- b) NCI from National Cancer Institute
- c) CCDC from Cambridge Crystallographic Data Center
- d) CAST from Chemical Abstract Service
- e) Derwent from Derwent Information Limited
- 5 f) Maybridge from Maybridge Chemical Company LTD
  - g) Aldrich from Aldrich Chemical Company
  - h) Directory of Natural Products from Chapman & Hall

One such data base (ACD distributed by Molecular Designs
Limited Information Systems) contains, for example,
200,000 compounds that are synthetically derived or are
natural products. Methods available to those skilled in
the art can convert a data set represented in two
dimensions to one represented in three dimensions.

These methods are enabled by such computer programs as CONCORD from Tripos Associates or DB-Converter from Molecular Simulations Limited.

Multiple methods of structure-based modulator design are known to those in the art. Kuntz et al., 1982, J. Mol. Biol. 162: 269; Kuntz et al., 1994, Acc. Chem. Res. 27: 117; Meng et al., 1992, J. Compt. Chem. 13: 505; Bohm, 1994, J. Comp. Aided Molec. Design 8: 623.

A computer program widely utilized by those skilled in the art of rational modulator design is DOCK from the University of California in San Francisco. The general methods utilized by this computer program and programs like it are described in three applications below. More detailed information regarding some of these techniques can be found in the Molecular Simulations User Guide, 1995.

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A typical computer program used for this purpose can comprise the following steps:

- (a) remove the existing compound from the protein;
- (b) dock the structure of another compound into the active-site using the computer program (such as DOCK) or by interactively moving the compound into the active-site;
- (c) characterize the space between the compound and the active-site atoms;
- (d) search libraries for molecular fragments which (i)can fit into the empty space between the compound and the active-site, and (ii) can be linked to the compound; and
  - (e) link the fragments found above to the compound and evaluate the new modified compound.

Part (c) refers to characterizing the geometry and the complementary interactions formed between the atoms of the active-site and the compounds. A favorable geometric fit is attained when a significant surface area is shared between the compound and active-site atoms without forming unfavorable steric interactions.

One skilled in the art would note that the method can be performed by skipping parts (d) and (e) and screening a data base of many compounds.

Structure-based design and identification of modulators of PTK function can be used in conjunction with assay screening. As large computer data base of compounds (around 10,000 compounds) can be searched in a matter of hours, the computer based method can narrow the compounds tested as potential modulators of PTK function in cellular assays.

The above descriptions of structure-based modulator design are not all encompassing and other methods are reported in the literature:

- (1) CAVEAT: Bartlett et al.,1989, in "Chemical and Biological Problems in Molecular Recognition", Roberts, S.M.; Ley, S.V.; Campbell, M.M. eds.; Royal Society of Chemistry: Cambridge, ppl82-196.
  - (2) FLOG: Miller et al., 1994, J. Comp. Aided Molec. Design 8:153.
- 10 (3) PRO Modulator: Clark et al., 1995, J. Comp. Aided Molec. Design 9:13.
  - (4) MCSS: Miranker and Karplus, 1991, Proteins: Structure, Function, and Genetics 11:29.
- (5) AUTODOCK: Goodsell and Olson, 1990, Proteins:15 Structure, Function, and Genetics 8:195.
  - (6) GRID: Goodford, 1985, J. Med. Chem. 28:849.

Design by Modifying Compounds in Complex with PTKs
Another way of identifying compounds as potential

modulators is to modify an existing modulator in the polypeptide active-site. For example, the computer representation of modulators can be modified within the computer representation of a PTK active-site. Detailed instructions for this technique can be found in the

Molecular Simulations User Manual, 1995 in LUDI. The computer representation of the modulator is modified by the deletion of a chemical group or groups or by the addition of a chemical group or groups.

Upon each modification to the compound, the atoms

of the modified compound and active-site can be shifted in conformation and the distance between the modulator

and the active-site atoms may be scored along with any complimentary interactions formed between the two molecules. Scoring can be complete when a favorable geometric fit and favorable complementary interactions are attained. Compounds that have favorable scores are potential modulators of PTK function.

# Design by Modifying the Structure of Compounds that Bind PTKs

10 A third method of structure-based modulator design is to screen compounds designed by a modulator building or modulator searching computer program. Examples of these types of programs can be found in the Molecular Simulations Package, Catalyst. Descriptions for using this program are documented in the Molecular Simulations User Guide (1995). Other computer programs used in this application are ISIS/HOST, ISIS/BASE, ISIS/DRAW) from Molecular Designs Limited and UNITY from Tripos Associates.

These programs can be operated on the structure of a compound that has been removed from the active-site of the three dimensional structure of a compound-PTK complex. Operating the program on such a compound is preferable since it is in a biologically active conformation.

A modulator construction computer program is a computer program that may be used to replace computer representations of chemical groups in a compound complexed with a PTK with groups from a computer data base. A modulator searching computer program is a computer program that may be used to search computer

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representations of compounds from a computer data base that have similar three dimensional structures and similar chemical groups as compound bound to a PTK.

A typical program can operate by using the following general steps:

- (a) map the compounds by chemical features such as by hydrogen bond donors or acceptors, hydrophobic/lipophilic sites, positively ionizable sites, or negatively ionizable sites;
- (b) add geometric constraints to the mapped features; and
  - (c) search data bases with the model generated in (b).

Those skilled in the art recognize that for indolinones, the important chemical features include, but are not limited to, a hydrogen bond donor, a hydrogen bond acceptor, and two hydrophobic points of contact. Those skilled in the art also recognize that not all of the possible chemical features of the compound need be present in the model of (b). One can use any subset of the model to generate different models for data base searches.

### IX. Organic Synthetic Techniques

The versatility of computer-based modulator design and identification lies in the diversity of structures screened by the computer programs. The computer programs can search data bases that contain 200,000 molecules and can modify modulators already complexed with the enzyme with a wide variety of chemical

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functional groups. A consequence of this chemical diversity is that a potential modulator of PTK function may take a chemical form that is not predictable. A wide array of organic synthetic techniques exist in the art to meet the challenge of constructing these potential modulators of PTK function. Many of these organic synthetic methods are described in detail in standard reference sources utilized by those skilled in the art. One example of such a reference is March, 1994, Advanced Organic Chemistry: Reactions, Mechanisms, and Structure, New York, McGraw Hill. Thus, the techniques required to synthesize a potential modulator of PTK function identified by computer-based methods are readily available to those skilled in the art of organic chemical synthesis.

### X. <u>Cellular Assays Measuring the Effect of a PTK</u> <u>Modulator in Signal Transduction Pathways</u>

20 Cellular assays can be used to test the activity of a potential modulator of PTK function as well as diagnose a disease associated with inappropriate PTK activity. A potential modulator of PTK function can be tested for activity in vitro by assays that measure the 25 effect of a potential modulator on the autophosphorylation of a particular PTK over-expressed in a cell line. Thus, a modulator that acts as a potent inhibitor of the catalytic domain corresponding to a PTK would decrease the amount of autophosphorylation 30 catalyzed by that PTK. Potential modulators could also be tested for activity in cell growth assays in vitro as well as in animal model assays in vivo.

In vivo assays are also useful for testing the bioactivity of a potential modulator designed by the methods of the invention.

Materials, methods, and experimental data for these assays are fully described in WO 96/40116 published on December 19, 1996, entitled "Indolinone Compounds for the Treatment of Disease". This application is incorporated herein by reference in its entirety, including all drawings, figures, and tables.

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# XI. Administration of Modulators of PTK Function as Therapeutics for Disease

Methods of administering compounds to organisms as therapeutics for disease are fully described in WO 96/40116 published on December 19, 1996, entitled "Indolinone Compounds for the Treatment of Disease". This application is incorporated herein by reference in its entirety, including all drawings, figures, and tables.

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#### **EXAMPLES**

The examples below are non-limiting and are merely representative of various aspects and features of the present invention. The examples provide illustrative methods for obtaining crystalline forms of protein kinase polypeptides, methods for determining three dimensional structures of these protein kinase polypeptides, and methods for identifying modulators of protein kinases using the three dimensional structures of the protein kinases.

### EXAMPLE 1: X-ray Crystallographic Structure Determination of FGFR1

#### Polypeptide Synthesis and Isolation

5 A recombinant baculovirus was engineered to encode residues 456-765 of human FGFR1. A cleavable N-terminal histidine tag was incorporated to aid in protein purification. Three amino acid substitutions were introduced: Cys-488 to Ala, Cys-584 to Ser and Leu-457 10 to Val. The two cysteine substitutions were made to prevent the formation of disulfide-linked oligomers. which occurs for the native protein. The substitution Leu-457 to Val introduced a Ncol cloning site near Met-456. The codon for Tyr-766 (TAC) was changed to a stop 15 codon (TAG) and a HindIII-cloning site was generated following this stop codon. These substitutions were introduced into the full length human cDNA of FGFR1 in m13MPI9 by site-directed mutagenesis according to the manufacturer's protocol (Amersham).

The resulting construct was digested with *Ncol* and *HindIII* and was ligated into appropriately digested pBlueBac HistagB (Invitrogen). Transfection of insect cells (Sf9) was performed with the BaculoGold transfection system according to the manufacturer's protocol (Pharmingen). Following identification of positive plaques, the recombinant baculovirus was amplified to high titer (5x10<sup>7</sup> virus particles/ml). Sf9 cells were grown in 175-cm<sup>2</sup> flasks to a density of 2-3x10<sup>7</sup> per flask and infected with recombinant baculovirus with a multiplicity of infection (MOI) of 10.

After 48 hr, cells were harvested by centrifugation

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at 3,000g for 35 min at 4°C and then lysed in 25 mM HEPES (pH 7.5), 150 mM NaCl, 10% glycerol, 1.5 mM MgCl<sub>2</sub>. 1 % Triton X-100, 10 µg/ml aprotonin, 10 µg/ml leupeptin, and 1 mM phenylmethylsulfonyl fluoride (PMSF). Lysates were centrifuged in a Sorval RC 5C (Dupont) for 1 hr at 4°C at 40,000g followed by ultracentrifugation in an XL-80 (Beckman) at 100,000g for 1 hr. After centrifugation, the clarified lysate was passed over a Ni<sup>2+</sup> -chelating column (Pharmacia), and the bound histidine-tagged fusion protein was eluted with 100 mM imidazole (pH 7.5). Pooled fractions were loaded onto a Mono Q anion exchange column (Pharmacia) and eluted with a NaCl gradient from 0 to 500 mM.

The fractions containing the fusion protein were 15 concentrated in a Centricon-30 (Amicon), and the histidine tag was removed by overnight digestion with enterokinase (Biozyme) at 20°C. The digestion was terminated by the addition of aprotonin, leupeptin, PMSF, TPCK, and bovine pancreatic trypsin inhibitor (BPTI). The cleaved kinase domain was then separated 20 from the histidine tag on a Superose 12 size-exclusion column (Pharmacia). The eluted kinase domain was further purified on a Mono Q column. The purified kinase domain was analyzed by N-terminal sequencing and mass spectrometry. Five amino acids (SAAGT) remained 25 from the histidine tag. The predicted molecular mass was confirmed by mass spectrometry.

#### Crystal Growth

Purified FGFR1 was concentrated to 20-50 mg/ml and exchanged into 10 mM Tris-HCl (pH 8.0), 10 mM NaCl, and

2 mM DTT using a Centricon-30. Crystals were grown at  $4\,^{\circ}$ C by vapor diffusion in hanging drops containing 2.0  $\mu$ l of 10 mg/ml protein solution and 2.0  $\mu$ l of reservoir solution: 16% polyethylene glycol (PEG) 10000, 0.3 M (NH,),SO,, 5% ethylene glycol, and 100 mM bis-Tris (pH 6.5).

Crystals of native FGFR1 were soaked in 500 ml stabilizing solution [25% PEG 10000, 0.3 M (NH4)<sub>2</sub>SO<sub>4</sub>, 0.1 M Bis-Tris (pH 6.5), 5% ethylene glycol] containing 3
[(3-(2-carboxyethyl)-4-methylpyrrol-5-yl)methylene]-2-indolinone (1-5 mM) or 3-[4-(4-formylpiperazine-1-yl)-benzylidenyl]-2-indolinone (1 mM) at 4°C for 24 to 48 hours. The final soaking concentration of DMSO was between 1 to 5%. The crystals cracked at higher concentrations of DMSO.

Co-crystals of FGFR1 with the inhibitors could also be obtained by vapor diffusion in hanging drops containing 2.0  $\mu$ l of 10 mg/ml protein solution and 2.0  $\mu$ l of reservoir solution containing 1 mM 3-[(3-(2-carboxyethyl)-4-methylpyrrol-5-yl)methylene]-2-indolinone and 3-[4-(4-formylpiperazine-1-yl-)benzylidenyl]-2-indolinone.

Co-crystals of FGFR1 complexed with AMP-PCP were obtained as described for the creation of native crystals, except that the protein solution additionally contained 10 mM AMP-PCP and 20 mM MgCl<sub>2</sub>.

#### Preparation Of Heavy Atom Derivative Crystals

Heavy atom derivative crystals were obtained by soaking FGFR1 native crystals (C2-A form) in a solution containing ethylmercurithiosalicylic acid (thimerosal),

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KAu(CN)<sub>2</sub> or 4-chloromercuribenzoic acid, as provided in Table 1, infra,, and containing 25% PEG 10000, 0.3M (NH<sub>4</sub>)<sub>2</sub>SO<sub>4</sub>, 5% ethylene glycol or glycerol, and 100 mM bis-Tris (pH 6.5), and were flash-cooled either in liquid nitrogen directly (Synchrotron) or in a dry nitrogen stream at -175°C (rotating anode).

# Data Collection and Structure Determination

For native crystals and crystals comprising the

nucleotide analog AMP-PCP, data were collected either on
a Rigaku RU-200 rotating anode operated at 50 kV and 100
mA (Cu Kα) and equipped with double-focusing mirrors and
an R-AXIS IIC image plate detector, or at beamline X-4A
at the National Synchrotron Light Source, Brookhaven

National Laboratory. Synchrotron data (λ=1.07Å) were collected on Fuji image plates and read with a Fuji scanner. One cryo-cooled crystal was used for each of the data sets. To obtain cryo-cooled crystals, crystals were soaked in a cryo-protectant solution containing 25%

PEG 10000, 0.3 M (NH<sub>4</sub>)<sub>2</sub>SO<sub>4</sub>, 5% ethylene glycol or glycerol and 100 mM bis-Tris (pH 6.5), and were flash-cooled either in liquid nitrogen directly (synchrotron data) or in a dry nitrogen stream at -175°C (rotating anode data). All data were processed using DENZO and

SCALEPACK. Otwinowski, 1993, "Oscillation data reduction program," Proceedings of the CCP4 Study Weekend, Sawyer et al., eds. (Daresbury, United Kingdom: SERC Daresbury Laboratory), 56-62.

For native crystals and crystals comprising the nucleotide analog AMP-PCP, a molecular replacement solution was found initially for the C2-B crystal form

using an IRK search model that consisted of polyalanine with the common side chains for residues 993-1263 (FGFR1 residues 475-754), excluding residues 1094-1105 (kinase insert) and 1153-1170 (activation loop). With AMORE 5 (Navaza, 1994, AmoRe: an automated package for molecular replacement," Acta Crystallogr. A50: 157-163), using 80% of the structure factor amplitudes between 15.0 and 3.5 A, one of the two molecules in the asymmetric unit was located. The correlation coefficient (c.c.) for the 10 correct 1-molecule solution was 0.23 (versus 0.20 for the highest incorrect solution). This molecule was rigid body-refined in X-PLOR (Brünger, 1992, X-PLOR (Version 3.1) Manual (New Haven, Conneticut: The Howeard Hughes Medical Institute and Department of Molecular 15 Biophysics and Biochemistry, Yale Uiversity)), first as one rigid body unit, then as two units each comprising a lobe of the kinase. Rigid body refinement (12.0-3.5 Å, F>30) resulted in a relative rotation of the two lobes of ~10° and an increase of the c.c. from 0.20 to 0.25. 20 The rigid body-refined molecule was then used as a new search model in AMORE, and this time both molecules in the asymmetric unit were located. The c.c. for the correct 2-molecule solution was 0.35 (versus 0.27 for the highest incorrect solution).

Multiple cycles of model building and refinement against 6.0-2.4 Å data resulted in the addition to the model of many of the side chains and some of the missing polypeptide chain. Model building was performed using TOM/FRODO (Jones, 1985, "Diffraction methods for biological macromolecules. Interactive computer graphics: FRODO," Methods in Enzymology 115: 157-171)

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and conjugate-gradient minimization and simulated annealing were performed using X-PLOR. Brünger, supra. At this stage, the R-value was 30% (free R-value of 36%). To help expedite model building and refinement, experimental phases were obtained. Because crystals grown in the presence of ethylene glycol were easier to manipulate than those grown in glycerol, several heavy-atom derivative data sets were collected from C2-A crystals that had been soaked in various heavy atom solutions. The C2-B structure was subsequently refined against 6.0-2.4 Å data to an R-value of 23.8% (free R-value of 30.4%) with r.m.s.d. values of 0.008 Å for bond distances and 1.4° for bond angles

Molecular replacement was used to locate the two 15 FGFR1 molecules (designated FLGK-A and FLGK-B) in the asymmetric unit of the C2-A crystal form. Using AMORE with 80% of structure factor amplitudes between 15.0 and 3.5 Å and the C2-B model, the c.c. for the correct 2molecule solution was 0.62 (versus 0.35 for the highest 20 incorrect solution). Heavy atom positions were determined from difference Fourier maps using the calculated phases from the partial model. Refinement of heavy atom parameters and phase determination were performed with MLPHARE (Otwinowski, 1991, "Maximum 25 likelihood refinement of heavy atom parameters," Isomorphous replacement and anomolous Ssattering, Evans and Leslie eds. (Darsbury, United Kingdom: SERC Daresbury Laboratory), 56-62)). An initial molecular isomorphous replacement (MIR)-phased electron density map was calculated with data between 2.0. and 2.8  $\hbox{\normale}{\normalfont{A}}$ 30 resolution. This map was improved by solvent

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flattening, histogram matching, and non-crystallographic symmetry (NCS) averaging using DM (Cowtan, 1994, "Protein Crystallography," CCP4 and ESF-EACBM Newsletter (joint) 31: 34-38).

Refinement of the C2-A FGFR1 structure against 6.0-2.0 Å data proceeded by conjugate-gradient minimization and simulated annealing using X-PLOR. Tight NCS restraints were imposed until data to 2.0 Å resolution were included in the refinement, at which point the restraints were lifted. An overall anisotropic B-value was calculated using X-PLOR and applied to the observed structure factors, reducing the R-value by ~3%. molecules whose B-values refined to ≥70 Ų were omitted from the subsequent refinement round. The average Bvalue is 37.5  $\mbox{Å}^2$  for all protein atoms, 35.4  $\mbox{Å}^2$  for protein atoms in FLGK-A,  $39.7 \ {\rm \AA}^2$  for protein atoms in FLGK-B, and 40.2 Å<sup>2</sup> for water molecules. The side chains for Cys-603 in FLGK-A and FLGK-B and for Met-534 in FLGK-B have been modeled in two different conformations. Residues that are not included in the atomic model due to poor supporting electron density are for FLGK-A: 456-463, 486-490, 501-504, 580-591, 763-765; and for FLG-B: 456-460, 501-504, 578-593, 646-651, 657-659, 762-765.

The positions of the two AMP-PCP molecules (one per FGFR1 molecule) were easily identified in  $2F_{\text{obs}(\text{co-complex})}$ -  $F_{\text{calc}(\text{FGPR})}$  difference Fourier maps. The AMP-PCP molecule bound to FLGK-B is less tightly bound and has been modeled with an occupancy of 0.5.

Table A summarizes the X-ray crystallography data

sets of FGFR1 derivative crystals that were used to

determine the structures of crystalline FGFR1 and



100 crystalline FGFR1:AMP-PCP co-complex of the invention.

TABLE 5

	Data Collection and MIR Phasing Summary							
	V ****	Native	AMP-PCP	Thi-12	Thi-2*	PCMB <sup>a</sup>	KAu(CN)	
	X-ray source	X-4A	RU-200	RU-200	RU-200	RU-200		
	Resolution limit (Å)	2.0	2.3	2.6	2.8		RU-200	
	Number of sites			4	7	2.8	2.8	
	Conc. (mM)/time (h)					2	2	
	R <sub>sym</sub> b(%)	4.8(19.7)°	4 5/22 236	0.1/24	0.1/48	0.2/2	5.0/72	
	Total observations	122569	4.5(23.3)°	5.5	9.8	6.8	6.8	
	Unique reflections		91324	55456	59488	67988	45303	
	Completeness (%)	50771	31997	42820 <sup>d</sup>	35538d	18619	18202	
		97.3(96.3) <sup>c</sup>	95.5(93.7)°	95.0	96.7	98.0	97.7	
	Signal (%1>3σ)	80.7(50.3) <sup>c</sup>	79.6(51.7)°	69.8	66.8	84.7	77.6	
	R <sub>iso</sub> e(%)		3.5.	17.1				
	Phasing power <sup>r</sup>				31.2	15.4	15.2	
	R <sub>cullis</sub> g(%)			1.8	2.0	1.0	0.9	
	Overall FOMh			0.55	0.50	0.81	0.84	

<sup>\*</sup>Thi-1, Thi-2; ethylmercurithiosalicylic acid (thimerosal); PCMB: 4-chloromercuribenzoic acid.

 $^eR_{iso} = 100 \text{ x } \Sigma_h \text{ [[F_p(h)\pm F_p(h)]-[F_{PH}(h)][/$\Sigma_h$]} F_p(h)], \text{ where } F_p \text{ and } F_{PH} \text{ are the native and derivative } F_p(h) = 100 \text{ m} \text{ for } F_p(h) = 100 \text{ m} \text{ fo$ structure factors, respectively.

Phasing power: r.m.s. heavy atom structure factor / r.m.s. lack of closure (for acentric reflections from 20.0 to 2.8Å).

30  ${}^gR_{cullis} = 100 \times \Sigma_h \left| \left| F_{PH}(h) \right| - F_{H(calc)}(h) \right| / \Sigma_h \left| F_{PH}(h) \pm F_p(h) \right| \text{ (for centric reflections from 20.0 to 2.8Å)}.$ <sup>h</sup>Figure of merit:  $\int P(\phi) \exp(i\phi) d\phi / \int P(\phi) d(\phi)$ , where P is the probability distribution of the phase angle φ.

 $<sup>{}^{</sup>b}R_{sym} = 100 \times \Sigma_{h}\Sigma_{i} | I_{i}(h) - \langle I(h) \rangle | / \Sigma_{h}\Sigma_{i}I_{i}(h)$ 

<sup>&</sup>lt;sup>c</sup>Value in parentheses is for the highest resolution shell.

<sup>&</sup>lt;sup>d</sup>I(+h) and I(-h) processed as independent reflections. Anomalous scattering contributions were included.

For crystals comprising FGFR1 and compounds 1 and 2, data were collected on a Rigaku RU-200 rotating anode (Cu Kα) operating at 50 kV and 100 mA and equipped with double-focusing mirrors and an R-AXIS IIC image plate detector. One cryo-cooled crystal was used for each of the data sets. Crystals were soaked in a cryo-protectant [25% PEG 10000, 0.3 M (NH.),SO., 5% ethylene glycol, 100 mM bis-Tris (pH 6.5), and 1 mM: [(3-(2-carboxyethy1)-4-methylpyrrol-5-y1)methylene]-2indolinone (hereafter referred to as compound 1) or 3-[4-(4-formylpiperazine-1-yl-)benzylidenyl]-2-indolinone (hereafter referred to as compound 2) and flash-cooled in a dry nitrogen stream at -175°C. Data were processed using DENZO and SCALEPACK. Otwinowski, 1993, Proceedings of the CCP4 Study Weekend (Daresbury, United Kingdom: SERC Daresbury Laboratory) pp 56-62.

A summary of the data collection parameters are included in the following Table 6:

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TABLE 6

	Resolution limit (Å)	Observa- tions (N)	Complete- ness (%)	Redundan- cy	R <sub>sym</sub> <sup>a</sup> (%)	Signal (I> ol)
compound 1	2.5	93535	97.6 (96.1)	2.7	6.8 (23.0)	11.8
compound	2.4	94093	99.1 (97.9)	3.3	6.3 (32.2)	11.4

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compound 1 structure: 550 residues, 252 water molecules, 2 compound 1 molecules (4589 atoms) compound 2 structure: 550 residues, 248 water molecules, 2 compound 2 molecules (4646 atoms)

#### 30 Structure Analyses

Atomic superpositions were performed with TOSS



(Hendrickson, 1979). Per residue solvent accessible surface calculations were done with X-PLOR. The surface area buried in a dimer interface was calculated with GRASP (Nicholls et al., 1991) using a probe radius of 1.4 Å. The stereochemical quality of the atomic model was monitored using PROCHECK (Laskowski et al., 1993, PROCHECK: a computer program to check the stereochemical quality of protein structures," J. Appl. Cryst. 26: 283-291). As defined in PROCHECK, 93% of the residues in the model have main-chain torsion angles in the most favored Ramachandran regions. There are no residues in disallowed regions, and three residues in generously allowed regions: Arg-622 in FLGK-A and FLGK-B and Arg-554 in FLGK-A. The overall G-factor score is 0.42.

Table 7 summarizes the X-ray crystallography refinement parameters of the structures of crystalline FGFR1 and crystalline FGFR1:AMP-PCP co-complex of the invention. Table 8 summarizes the X-ray crystallography refinement parameters for the FGFR1/compound complexes.

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TABLE 7

Refinement Parameters  FGFR1: 550 residues, 252 water molecules (4589 atoms)  FGFR1:AMP-PCP: 550 residues, 238 water molecules, 2 AMP-PCP molecules (4638 atoms)  Model d-spacings Reflection Parameters								
	(Å)	(N)	(%)	bonds (Å)	angles (°)	B-values		
FGFR1:	6.0-2.0	42548	21.3 (26.2)°	^ ^ ^ -		(Ų)		
FGFR1:AMP-PCP:	6.0-2.3	26729	20.1 (27.5) <sup>c</sup>	0.008	1.3	1.6		

<sup>a</sup>R-value = 100 x  $\Sigma_h$   $||F_{obs}(h)| - |F_{calc}(h)|| / \Sigma_h |F_{obs}(h)|$  for reflections with  $F_{obs} > 2\sigma$ .

TABLE 8

Model	d-spacings (Å)	Reflec- tions	R- value' (N)	bonds (Å)	angles (°)	B- values <sup>(</sup> (Å <sup>2</sup> )
compound l	6.0-2.4	42548	19.7 (27.0) <sup>k</sup>	0.008	1.3	1.6
compound 2	6.0–2.5	26729	20.0 (28.0) <sup>k</sup>	0.008	1.4	1.7

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15 For bonded protein atoms.

#### Atomic Structural Coordinates

Tables 1 and 2 provide the atomic structural 20 coordinates of unphosphorylated FGFR1 and unphosphorylated FGFR1:AMP-PCP co-complex, respectively. In the Tables, coordinates for both of the FGFR1 molecules of the dimer comprising the asymmetric unit are provided. The amino acid residue numbers coincide 25 with those used in FIG. 3. In the first FGFR1 molecule of the dimer the residue number is preceded by a 1, i.e., residue number 464 of the first FGFR1 molecule of the dimer is denoted by "1464". Tables 3 and 4 provide the atomic structural coordinates of FGFR1 in complex 30 with indolinone compounds found to inhibit FGFR1 function.

<sup>&</sup>lt;sup>b</sup>For bonded protein atoms.

<sup>&#</sup>x27;Value in parentheses is the free R-value (Brünger, 1993) determined from 5% of the data.

 $<sup>{}^{</sup>a}R_{sym} = 100 \times S_{h}S_{i} |I_{i}(h) - I(h)^{0}| / S_{h}S_{i} I_{i}(h)$ 

<sup>&</sup>quot;Value in parentheses is for the highest resolution shell.

<sup>&</sup>lt;sup>i</sup>R-value = 100 x S<sub>h</sub>  $||F_o(h)| - |F_c(h)|| / S_h |F_o(h)|$ , where  $F_o$  and  $F_c$  are the observed and calculated structure factors, respectively  $(F_o > 2s)$ .

<sup>\*</sup>Value in parentheses is the free R-value determined from 5% of the data.

The following abbreviations are used in the Tables:

"Atom Type" refers to the element whose coordinates are provided. The first letter in the column defines the element.

5 "A.A." refers to amino acid.

"X, Y and Z" provide the Cartesian coordinates of the element.

"B" is a thermal factor that measures movement of the atom around its atomic center

"OCC" refers to occupancy, and represents the percentage of time the atom type occupies the particular coordinate. OCC values range from 0 to 1, with 1 being 100%

"PRT1" or "PRT2" relate to occupancy, with PRT1

designating the coordinates of the atom when in the

first conformation and PRT2 designating the coordinates

of the atom when in the second or alternate

conformation.

Structural coordinates for FGFR1 may be modified by
mathematical manipulation. Such manipulations include,
but are not limited to, crystallographic permutations of
the raw structure coordinates, fractionalization of the
raw structure coordinates, integer additions or
subtractions to sets of the raw structure coordinates,
inversion of the raw structure coordinates and any
combination of the above

In addition, the structural coordinates can be slightly modified and still render nearly identical three dimensional structures. Therefore, a measure of a unique set of structural coordinates is the root-mean-square deviation of the resulting structure. Structural

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coordinates that render three dimensional structures that deviate from one another by a root-mean-square deviation of less than 1.5 Å may be viewed as identical.

### 5 <u>EXAMPLE 2</u>: <u>Computer-Based Design of Modulators of PTK Function</u>

Potential modulators of PTK function were designed and identified by operating the program Catalyst on the structure of 3-[(3-(2-carboxyethyl)-4-methylpyrrol-5-yl)methylene]-2-indolinone. The chemical features constraining the search model include a hydrogen bond donor, a hydrogen bond acceptor, and two hydrophobic points of contact. Approximately 40 compounds were identified as potential modulators of PTK function using this method.

The compounds identified by the method as potential modulators of PTK function were commercially available. These compounds were then tested for their ability to inhibit the FLK PTK in an enzyme linked immunosorbant assay (ELISA). The method of performing this assay is taught in WO 96/40116, entitled "Indolinone Compounds for the Treatment of Disease," published on December 19, 1996, invented by Tang et al., incorporated by reference herein in its entirety, including all figures, drawings, and tables. Flk-1 specific antibodies can be prepared from the following protocol:

Prepare a Tresyl-Activated Agarose/Flk-1-D column
 by incubating 10 ml of Tresyl-Activated Agarose
 with 20 mg of purified GST-Flk-1-D fusion protein

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in 100mM sodium bicarbonate (pH 9.6) buffer overnight at 4°C.

- 2. Wash the column once with PBS.
- 3. Block the excess sites on the column with 2  $\mbox{M}$ glycine for 2 hours at 4°C.
- Wash the column with PBS. 4.
- 5. Incubate the column with Rabbit anti-Flk-1D production bleed for 2 hours at 4°C.
- 6. Wash the column with PBS.
- 10 7. Elute antiserum with 100 mM Citric Acid, pH3.0 and neutralize the eluate immediately with 2 M Tris, pH 9.0.
  - Dialyize the eluate against PBS overnight at 4oC 8. with 3 changes of buffer (sample to buffer ratio is 1:100).
  - 9. Adjust the dialyized antiserum to 5% glycerol and store at -80°C in small aliquotes.

The Flk-1 ELISA can include a 2,2-azino-bis(3-20 ethylbenz-thiazoline-6-sulfonic acid (ABTS) solution, which can comprise 100mM citric acid (anhydrous), 250 mM  $\mathrm{Na_2HPO_4}$  (pH 4.0), 0.5 mg/ml ABTS (Sigma catalog no. A-The solution is most appropriately stored in dark at 4°C until ready for use.

25 The FLK-1 specific antibodies can also be purchased from Santa Cruz Biotechnology (Catalog No. SC-504).

Four of the forty compounds identified as potential modulators of PTK function were potent modulators of FLK function. These molecules have the following

30 structures:

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The modulators inhibit the FLK protein kinase with the following  $IC_{50}$  values:

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TABLE 9

Compound	FLK kinase	FLK kinase	EGFR	IGF-1R
	IC <sub>50</sub>	IC <sub>so</sub>	IC <sub>50</sub>	IC <sub>50</sub>
	(μM)	(μM)	(μM)	(μM)
	compounds	compounds	·	
	tested at 100µM	tested at 20µM		
1	14.8	14	>100	>100
2	15.7	10.6	>100	>100
3	21.4	16.6	68	30.9
4	22.9	16.4	>100	>100

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The invention illustratively described herein may be practiced in the absence of any element or elements, limitation or limitations which is not specifically disclosed herein. The terms and expressions which have

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been employed are used as terms of description and not of limitation, and there is no intention that in the use of such terms and expressions of excluding any equivalents of the features shown and described or portions thereof, but it is recognized that various modifications are possible within the scope of the invention claimed. Thus, it should be understood that although the present invention has been specifically disclosed by preferred embodiments and optional features, modification and variation of the concepts herein disclosed may be resorted to by those skilled in the art, and that such modifications and variations are considered to be within the scope of this invention as defined by the appended claims.

Those references not previously incorporated herein by reference, including both patent and non-patent references, are expressly incorporated herein by reference for all purposes. Other embodiments are within the following claims.

WO 98/07835 PCT/US97/14885

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#### SEOUENCE LISTING

### (1) GENERAL INFORMATION:

(i) APPLICANT: SUGEN, INCORPORATED

351 Galveston Drive Redwood City, CA 94063

(ii) TITLE OF INVENTION: CRYSTAL STRUCTURES OF A

PROTEIN TYROSINE KINASE

(iii) NUMBER OF SEQUENCES: 5

(iv) CORRESPONDENCE ADDRESS:

(A) ADDRESSEE: Lyon & Lyon

(B) STREET: 633 West Fifth Street

Suite 4700

(C) CITY: Los Angeles

(D) STATE: California

(E) COUNTRY: U.S.A.

(F) ZIP: 90071-2066

(v) COMPUTER READABLE FORM:

(A) MEDIUM TYPE: 3.5" Diskette, 1.44 Mb

storage

(B) COMPUTER: IBM Compatible

(C) OPERATING SYSTEM: IBM P.C. DOS 5.0
(D) SOFTWARE: Fast SEO for Winds

(D) SOFTWARE: FastSEQ for Windows 2.0

(vi) CURRENT APPLICATION DATA:

(A) APPLICATION NUMBER: To Be Assigned

(B) FILING DATE: Herewith

(C) CLASSIFICATION:

(vii) PRIOR APPLICATION DATA:

(A) APPLICATION NUMBER:

(B) FILING DATE:

## (viii) ATTORNEY/AGENT INFORMATION:

(A) NAME:

Warburg, Richard J.

(B) REGISTRATION NUMBER:

32,327

(C) REFERENCE/DOCKET NUMBER: 227/088-PCT

# (ix) TELECOMMUNICATION INFORMATION:

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(213) 489-1600

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(C) TELEX:

67-3510

## (2) INFORMATION FOR SEQ ID NO:1:

## (i) SEQUENCE CHARACTERISTICS:

(A) LENGTH:

310 amino acids

(B) TYPE:

amino acid

(C) STRANDEDNESS:

single linear

(D) TOPOLOGY:

protein

(ii) MOLECULE TYPE:

(iii) HYPOTHETICAL:

NO

# (xi) SEQUENCE DESCRIPTION: SEQ ID NO:1:

Met Leu Ala Gly Val Ser Glu Tyr Glu Leu Pro Glu Asp Pro Arg Trp

Glu Leu Pro Arg Asp Arg Leu Val Leu Gly Lys Pro Leu Gly Glu Gly

Cys Phe Gly Gln Val Val Leu Ala Glu Ala Ile Gly Leu Asp Lys Asp 40

Lys Pro Asn Arg Val Thr Lys Val Ala Val Lys Met Leu Lys Ser Asp

Ala Thr Glu Lys Asp Leu Ser Asp Leu Ile Ser Glu Met Glu Met Met

Lys Met Ile Gly Lys His Lys Asn Ile Ile Asn Leu Leu Gly Ala Cys 90

Thr Gln Asp Gly Pro Leu Tyr Val Ile Val Glu Tyr Ala Ser Lys Gly

Asn Leu Arg Glu Tyr Leu Gln Ala Arg Arg Pro Pro Gly Leu Glu Tyr 120

Cys Tyr Asn Pro Ser His Asn Pro Glu Glu Gln Leu Ser Ser Lys Asp 135

Leu Val Ser Cys Ala Tyr Gln Val Ala Arg Gly Met Glu Tyr Leu Ala 145 150 155

Ser Lys Lys Cys Ile His Arg Asp Leu Ala Ala Arg Asn Val Leu Val 165 170

Thr Glu Asp Asn Val Met Lys Ile Ala Asp Phe Gly Leu Ala Arg Asp 180

Ile His His Ile Asp Tyr Tyr Lys Lys Thr Thr Asn Gly Arg Leu Pro 200

Val Lys Trp Met Ala Pro Glu Ala Leu Phe Asp Arg Ile Tyr Thr His 210 215

Gln Ser Asp Val Trp Ser Phe Gly Val Leu Leu Trp Glu Ile Phe Thr 230 235

Leu Gly Gly Ser Pro Tyr Pro Gly Val Pro Val Glu Glu Leu Phe Lys 245 250

Leu Leu Lys Glu Gly His Arg Met Asp Lys Pro Ser Asn Cys Thr Asn 260 265 270

Glu Leu Tyr Met Met Arg Asp Cys Trp His Ala Val Pro Ser Gln 275 280

Arg Pro Thr Phe Lys Gln Leu Val Glu Asp Leu Asp Arg Ile Val Ala

Leu Thr Ser Asn Gln Glu 305 310

#### (2) INFORMATION FOR SEQ ID NO:2:

#### (i) SEQUENCE CHARACTERISTICS:

(A) LENGTH:

315 amino acids

(B) TYPE:

amino acid

(C) STRANDEDNESS: single

(D) TOPOLOGY:

linear

(ii) MOLECULE TYPE:

protein

(iii) HYPOTHETICAL:

(xi) SEQUENCE DESCRIPTION: SEQ ID NO:2:

Ser Ala Ala Gly Thr Met Val Ala Gly Val Ser Glu Tyr Glu Leu Pro

Glu Asp Pro Arg Trp Glu Leu Pro Arg Asp Arg Leu Val Leu Gly Lys 25



- Pro Leu Gly Glu Gly Ala Phe Gly Gln Val Val Leu Ala Glu Ala Ile 35 40 45
- Gly Leu Asp Lys Asp Lys Pro Asn Arg Val Thr Lys Val Ala Val Lys
  50 55 60
- Met Leu Lys Ser Asp Ala Thr Glu Lys Asp Leu Ser Asp Leu Ile Ser 65 70 75 80
- Glu Met Glu Met Lys Met Ile Gly Lys His Lys Asn Ile Ile Asn 85 90 95
- Leu Leu Gly Ala Cys Thr Gln Asp Gly Pro Leu Tyr Val Ile Val Glu 100 105 110
- Tyr Ala Ser Lys Gly Asn Leu Arg Glu Tyr Leu Gln Ala Arg Arg Pro 115 120 125
- Pro Gly Leu Glu Tyr Ser Tyr Asn Pro Ser His Asn Pro Glu Glu Gln 130 135 140
- Leu Ser Ser Lys Asp Leu Val Ser Cys Ala Tyr Gln Val Ala Arg Gly
  145 150 155 160
- Met Glu Tyr Leu Ala Ser Lys Lys Cys Ile His Arg Asp Leu Ala Ala 165 170 175
- Arg Asn Val Leu Val Thr Glu Asp Asn Val Met Lys Ile Ala Asp Phe 180 185 190
- Gly Leu Ala Arg Asp Ile His His Ile Asp Tyr Tyr Lys Lys Thr Thr 195 200 205
- Asn Gly Arg Leu Pro Val Lys Trp Met Ala Pro Glu Ala Leu Phe Asp 210 215 220
- Arg Ile Tyr Thr His Gln Ser Asp Val Trp Ser Phe Gly Val Leu Leu 225 235 240
- Trp Glu Ile Phe Thr Leu Gly Gly Ser Pro Tyr Pro Gly Val Pro Val 245 250 255
- Glu Glu Leu Phe Lys Leu Leu Lys Glu Gly His Arg Met Asp Lys Pro 260 265 270
- Ser Asn Cys Thr Asn Glu Leu Tyr Met Met Met Arg Asp Cys Trp His 275 280 285
- Ala Val Pro Ser Gln Arg Pro Thr Phe Lys Gln Leu Val Glu Asp Leu 290 295 300
- Asp Arg Ile Val Ala Leu Thr Ser Asn Gln Glu 305 310 315

#### (2) INFORMATION FOR SEQ ID NO:3:

(i) SEQUENCE CHARACTERISTICS:

(A) LENGTH: 351 amino acids

(B) TYPE: amino acid

(C) STRANDEDNESS: single

(D) TOPOLOGY: linear

(ii) MOLECULE TYPE: protein

(iii) HYPOTHETICAL: NO

(xi) SEQUENCE DESCRIPTION: SEQ ID NO:3:

Met Arg Gly Ser His His His His His Gly Met Ala Ser Met Thr

10 15

Gly Gly Gln Gln Met Gly Arg Asp Leu Tyr Asp Asp Asp Asp Lys Asp 20 25 30

Pro Ser Ser Arg Ser Ala Ala Gly Thr Met Val Ala Gly Val Ser Glu 35 40 45

Tyr Glu Leu Pro Glu Asp Pro Arg Trp Glu Leu Pro Arg Asp Arg Leu 50 55 60

Val Leu Gly Lys Pro Leu Gly Glu Gly Ala Phe Gly Gln Val Leu 65 70 75 80

Ala Glu Ala Ile Gly Leu Asp Lys Asp Lys Pro Asn Arg Val Thr Lys
85 90 95

Val Ala Val Lys Met Leu Lys Ser Asp Ala Thr Glu Lys Asp Leu Ser

Asp Leu Ile Ser Glu Met Glu Met Met Lys Met Ile Gly Lys His Lys 115 120 125

Asn Ile Ile Asn Leu Leu Gly Ala Cys Thr Gln Asp Gly Pro Leu Tyr 130 135 140

Val Ile Val Glu Tyr Ala Ser Lys Gly Asn Leu Arg Glu Tyr Leu Gln 145 150 155 160

Ala Arg Arg Pro Pro Gly Leu Glu Tyr Ser Tyr Asn Pro Ser His Asn 165 170 175

Pro Glu Glu Gln Leu Ser Ser Lys Asp Leu Val Ser Cys Ala Tyr Gln 180 185 190

Val Ala Arg Gly Met Glu Tyr Leu Ala Ser Lys Lys Cys Ile His Arg 195 200 205 WO 98/07835 PCT/US97/14885

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Asp	Leu 210	Ala	a Ala	a Arç	Asn	Val 215	Leu	ı Val	Thi	Gli	220	Ası	n Val	l Met	Ly:
Ile 225	Ala	Asp	Phe	e Gly	Leu 230	Ala	Arg	Asp	) Ile	His 235	His	; Ile	e Asr	туг	Ty:
Lys	Lys	Thr	Thr	Asn 245	Gly	Arg	Leu	Pro	Val 250	Lys	Trp	Met	Ala	Pro 255	Glu
Ala	Leu	Phe	<b>As</b> p 260	Arg	Ile	Tyr	Thr	His 265	Gln	Ser	Asp	Val	Trp 270		Phe
Gly	Val	Leu 275	Leu	Trp	Glu	Ile	Phe 280	Thr	Leu	Gly	Gly	Ser 285		Tyr	Pro
Gly	Val 290	Pro	Val	Glu	Glu	Leu 295	Phe	Lys	Leu	Leu	Lys 300	Glu	Gly	His	Arg
Met 305	Asp	Lys	Pro	Ser	Asn 310	Суз	Thr	Asn	Glu	Leu 315	Tyr	Met	Met	Met	Arg 320
Asp	Cys	Trp	His	Ala 325	Val	Pro	Ser	Gln	Arg 330	Pro	Thr	Phe	Lys	Gln 335	Leu
Val (	Glu	Asp	Leu 340	Asp	Arg	Ile	Val	Ala 345	Leu	Thr	Ser	Asn	Gln 350	Glu	

### (2) INFORMATION FOR SEQ ID NO:4:

### (i) SEQUENCE CHARACTERISTICS:

(A) LENGTH: 933 base pairs
(B) TYPE: nucleic acid

(C) STRANDEDNESS: double (D) TOPOLOGY: linear

(ii) MOLECULE TYPE: cDNA to mRNA

### (xi) SEQUENCE DESCRIPTION: SEQ ID NO:4:

ATGCTAGCAG GGGTCTCTGA GTATGAGCTT CCCGAAGACC CTCGCTGGGA GCTGCCTCGG 60
GACAGACTGG TCTTAGGCAA ACCCCTGGGA GAGGGCTGCT TTGGGCAGGT GGTGTTGGCA 120
GAGGCTATCG GGCTGGACAA GGACAAACCC AACCGTGTGA CCAAAGTGGC TGTGAAGATG 180
TTGAAGTCGG ACGCAACAGA GAAAGACTTG TCAGACCTGA TCTCAGAAAT GGAGATGATG 240
AAGATGATCG GGAAGCATAA GAATATCATC AACCTGCTGG GGGCCTGCAC GCAGGATGGT 300
CCCTTGTATG TCATCGTGGA GTATGCCTCC AAGGGCAACC TGCGGGAGTA CCTGCAGGCC 360
CGGAGGCCCC CAGGGCTGGA ATACTGCTAC AACCCCAGCC ACAACCCAGA GGAGCAGCTC 420



TCCTCCAAGG	ACCTGGTGTC	CTGCGCCTAC	CAGGTGGCCC	GAGGCATGGA	GTATCTGGCC	480
TCCAAGAAGT	GCATACACCG	AGACCTGGCA	GCCAGGAATG	TCCTGGTGAC	AGAGGACAAT	540
GTGATGAAGA	TAGCAGACTT	TGGCCTCGCA	CGGGACATTC	ACCACATCGA	СТАСТАТААА	600
AAGACAACCA	ACGGCCGACT	GCCTGTGAAG	TGGATGGCAC	CCGAGGCATT	ATTTGACCGG	660
ATCTACACCC	ACCAGAGTGA	TGTGTGGTCT	TTCGGGGTGC	TCCTGTGGGA	GATCTTCACT	720
CTGGGCGGCT	CCCCATACCC	CGGTGTGCCT	GTGGAGGAAC	TTTTCAAGCT	GCTGAAGGAG	780
GGTCACCGCA	TGGACAAGCC	CAGTAACTGC	ACCAACGAGC	TGTACATGAT	GATGCGGGAC	840
TGCTGGCATG	CAGTGCCCTC	ACAGAGACCC	ACCTTCAAGC	AGCTGGTGGA	AGACCTGGAC	900
CGCATCGTGG	CCTTGACCTC	CAACCAGGAG	TAG			933

### (2) INFORMATION FOR SEQ ID NO:5:

#### (i) SEQUENCE CHARACTERISTICS:

(A) LENGTH: 1056 base pairs (B) TYPE: nucleic acid

(C) STRANDEDNESS: double

(D) TOPOLOGY: linear

(ii) MOLECULE TYPE: CDNA

### (xi) SEQUENCE DESCRIPTION: SEQ ID NO:5:

ATGCGGGGTT CTCATCATCA	A TCATCATCAT	GGTATGGCTA	GCATGACTGG	TGGACAGCAA	60
ATGGGTCGGG ATCTGTACGA	CGATGACGAT	AAGGATCCGA	GCTCGAGATC	TGCAGCTGGT	120
ACCATGGTAG CAGGGGTCTC	TGAGTATGAG	CTTCCCGAAG	ACCCTCGCTG	GGAGCTGCCT	180
CGGGACAGAC TGGTCTTAGG	CAAACCCCTG	GGAGAGGGCG	CCTTTGGGCA	GGTGGTGTTG	240
GCAGAGGCTA TCGGGCTGGA	CAAGGACAAA	CCCAACCGTG	TGACCAAAGT	GGCTGTGAAG	300
ATGTTGAAGT CGGACGCAAC	AGAGAAAGAC	TTGTCAGACC	TGATCTCAGA	AATGGAGATG	360
ATGAAGATGA TCGGGAAGCA	TAAGAATATC	ATCAACCTGC	TGGGGGCCTG	CACGCAGGAT	420
GGTCCCTTGT ATGTCATCGT	GGAGTATGCC	TCCAAGGGCA	ACCTGCGGGA	GTACCTGCAG	480
GCCCGGAGGC CCCCAGGGCT	GGAATACTCC	TACAACCCCA	GCCACAACCC	AGAGGAGCAG	540
CTCTCCTCCA AGGACCTGGT	GTCCTGCGCC	TACCAGGTGG	CCCGAGGCAT	GGAGTATCTG	600
GCCTCCAAGA AGTGCATACA	CCGAGACCTG	GCAGCCAGGA	ATGTCCTGGT	GACAGAGGAC	660



AATGTGATG	A AGATAGCAGA	CTTTGGCCTC	CC)CCCC		CGACTACTAT	
λλλλλα			GCACGGGACA	TTCACCACAT	CGACTACTAT	720
AAAAAGACAA	A CCAACGGCCG	ACTGCCTGTG	AAGTGGATGG	CACCCGAGGC	ATTATTTGAC	
CGGATCTACA	CCCACCAGAG	TC Macana			ATTATTTGAC	780
2.000		1GM1G1G1GG	TCTTTCGGGG	TGCTCCTGTG	GGAGATCTTC	840
ACTCTGGGCG	GCTCCCCATA	CCCCGGTGTG	CCTGTGGAGG	<b>ል ል ር ጥ</b> ጥጥጥ ለ አ		
GAGGGTCACC	GCATGGAGAA	2222		- LACITICAA	GCTGCTGAAG	900
	GCATGGACAA	GCCCAGTAAC	TGCACCAACG	AGCTGTACAT	GATGATGCGG	960
GACTGCTGGC	ATGCAGTGCC	CTCACAGAGA	CCCACCTTCA	ACCA COTA		200
GACCGCATCC	maaa		outleerich .	AGCAGCTGGT	GGAAGACCTG	1020
CCCCA1CG	TGGCCTTGAC	CTCCAACCAG	GAGTAG			
						1056



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### TABLE 1

Ato No		Atom Type	A.A	A.A No.	x	Y	Z	occ	В	
ATOM	1	N	GLU	1464	12 630	16 026	0. 521	1 00		
ATOM	3	CA	GLU	1464	-13.639	16.975	8.571	1.00	54.29	
ATOM	4	CB	GLU	1464	-12.479 -11.400	17.105	7.695	1.00	52.62	
ATOM	5	C		1464		17.974	8.349	1.00	54.64	
ATOM	6	0	GLU GLU	1464	-11.914	15.738	7.319	1.00	49.74	
ATOM	7	N	LEU	1464	-11.845	15.407	6.136	1.00	52.04	
ATOM	9	CA	LEU	1465 1465	-11.562 -11.018	14.925	8.310	1.00	44.95	
ATOM	10	CB	LEU	1465	-10.236	13.599	8.037	1.00	41.04	
ATOM	11	CG	LEU	1465	-8.719	13.066	9.235	1.00	40.18	
ATOM	12	CD1	LEU	1465	-8.346	13.196	9.130	1.00	43.70	
ATOM	13	CD2	LEU	1465	-8.061	14.654	8.891	1.00	46.74	
ATOM	14	CD2	LEU	1465	-12.092	12.671	10.395	1.00	40.72	
ATOM	15	0	LEU	1465	-12.032	12.594	7.656	1.00	39.18	
ATOM	16	N	PRO	1466	-11.802	12.590	8.219	1.00	38.05	
ATOM	17	CD	PRO	1466	-10.597	11.748	6.657	1.00	37.20	
ATOM	18	CA	PRO	1466	-12.741	11.793 10.727	5.810	1.00	36.41	
ATOM	19	CB	PRO	1466	-12.110		6.189	1.00	36.13	
ATOM	20	CG	PRO	1466	-10.629	10.262 10.459	4.878	1.00	37.50	
ATOM	21	C	PRO	1466	-12.846		5.135	1.00	36.20	
ATOM	22	0	PRO	1466	-11.847	9.595 9.174	7.201 7.788	1.00	35.61 35.18	
ATOM	23	N	GLU	1467	-14.060	9.121	7.429	1.00		
ATOM	25	CA	GLU	1467	-14.268	8.053	8.377	1.00	35.38 35.43	
ATOM	26	CB	GLU	1467	-15.744	7.965	8.746	1.00	41.10	
ATOM	27	CG	GLU	1467	-16.375	9.280	9.098	1.00	48.25	
ATOM	28	CD	GLU	1467	-17.819	9.145	9.596	1.00	50.24	
ATOM	29	OE1	GLU	1467	-18.446	8.071	9.378	1.00	52.82	
ATOM	30	OE2	GLU	1467	-18.314	10.109	10.230	1.00	51.26	
ATOM	31	C	GLU	1467	-13.838	6.714	7.801	1.00	32.65	
ATOM	32	Ō	GLU	1467	-13.899	6.511	6.591	1.00	35.06	
ATOM	33	N	ASP	1468	-13.299	5.854	8.659	1.00	30.46	
ATOM	35	CA	ASP	1468	-12.883	4.516	8.262	1.00	28.85	
ATOM	36	CB	ASP	1468	-11.384	4.424	7.975	1.00	29.34	
ATOM	37	CG	ASP	1468	-10.985	3.072	7.408	1.00	27.57	
ATOM	38	OD1	ASP	1468	-11.833	2.159	7.359	1.00	27.78	
MOTA	39	OD2	ASP	1468	-9.817	2.916	7.003	1.00	30.64	
ATOM	40	С	ASP	1468	-13,252	3.564	9.384	1.00	29.29	
ATOM	41	0	ASP	1468	-12.481	3.364	10.336	1.00	27.76	
ATOM	42	N	PRO	1469	-14.435	2.939	9.268	1.00	28.99	
ATOM	43	CD ·	PRO	1469	-15.354	3.091	8.120	1.00	28.09	
ATOM	44	CA	PRO	1469	-14.971	1.987	10.244	1.00	30.01	
ATOM	45	CB	PRO	1469	-16.244	1.473	9.553	1.00	33.33	
MOTA	46	CG	PRO	1469	-16.665	2.630	8.690	1.00	30.53	
ATOM	47	С	PRO	1469	-14.012	0.848	10.563	1.00	28.96	
ATOM	48	0	PRO	1469	-14.085	0.251	11.636	1.00	28.52	
ATOM	49	N	ARG	1470	-13.106	0.556	9.631	1.00	27.59	
ATOM	51	CA	ARG	1470	-12.139	-0.520	9.810	1.00	27.37	
ATOM	52	CB	ARG	1470	-11.301	-0.707	8.533	1.00	28.84	

A	TOM 5	3	CG	אמת								
A	<b></b> .				1470	0		-1.2	79 7.	317	1.00	30.55
	TOM 5	_ '	·		1470			-1.39		068	1.00	,
	TOM 5				L470		39	-0.06		793	1.00	
	TOM 5	•		. ~ ~	470	,	3	0.15		323		
	TOM 6	_			470	-9.24	11 .	-0.82			1.00	00
	rom 64	-	-		470	-9.06	7	1.35			1.00	33.19
	rom 6	. ~			470	-11.18	0 -	-0.28			1.00	28.65
	OM 66				470	-10.75		1.23			1.00	29.21
	OM 68				471	-10.90	9	0.97			1.00	28.47
	OM 69		_ ~		471	-9.94	0	1.31			1.00	27.80
АТ			_		471	-8.72		1.94			1.00	28.62
AT		•			171	-8.04		0.976			1.00	24.97
AT					171	-7.15		0.060			1.00	24.86
ATO		CI			171	-6.782		0.77 <i>6</i>	_		1.00	28.00
ATO		CE		RP 14	71	-6.642		0.460			1.00	29.23
ATO	· -	CI			71	-8.166		0.860			1.00	26.59
ATO		NE		RP 14	71	-7.413		0.192			1.00	27.23
ATO		CZ			71	-5.912		l . 866			1.00	30.10
ATO		CZ		P 14	71	-5.778		.545	_		1.00	28.70
ATO		CH	2 TR	P 14	71	-5.424	-	2.237			1.00	27.18
ATO		C	TR	P 14	71	-10.371		.223			.00	27.23
ATO		0	TR	P 14	71	-9.664			13.44		00	28.42
ATO		N	GL			-11.521		.321	14.44		.00	26.48
		CA	GL		72	-11.981		.874	13.29		.00	28.62
OTA OTA		CB	GLī	J 147	72	-13.245		.823	14.29		.00	27.16
		CG	GLt	J 147	2	-13.552		.534	13.799		.00	28.89
ATO		CD	GLU	147	2	-12.692		.869	14.520		.00	29.09
ATON	_	OE1	GLU	147		-12.134		.042	14.054		.00	26.43
ATON		OE2	GLU			-12.596		.009	12.938		.00	28.59
ATOM	- •	C	GLU	147		-12.217		024	14.801		.00	27.28
ATOM	<del>-</del>	0	GLU			-12.763		269	15.701		.00 ;	25.10
ATOM		N	LEU	147		-11.750		196	15.861	1.		26.48
ATOM	<del>-</del>	CA	LEU	147		-11.962		991	16.711	1.		24.65
ATOM		CB	LEU	147		10.645		608	18.104	1.		26.27
ATOM		CG	LEU	147		10.750		266	18.817	1.		8.24
ATOM		CD1	LEU	1473		11.323		025	20.337	1.		7.23
ATOM		CD2	LEU	1473		-9.390		636	20.642	1.		5.23
ATOM	99	C	LEU	1473		12.546		183	21.000	1.		6.33
ATOM	100	0	LEU	1473		12.122		856	18.740	1.0		6.52
ATOM	101	N	PRO	1474		13.610		973	18.411	1.0		5.16
ATOM	102	CD	PRO	1474		14.435	4.7		19.554	1.0	00 2	8.52
ATOM	103	CA	PRO	1474		14.215	3.5		19.770	1.0		9.65
ATOM	104	CB	PRO	1474		15.368	5.8		20.207	1.0		9.18
ATOM	105	CG	PRO	1474		15.768	5.2		21.003	1.0		3.58
ATOM	106	C	PRO	1474			4.0		20.154	1.0		3.17
MOTA	107	0	PRO	1474		13.173	6.5		21.124	1.0		7.75
MOTA	108	N	ARG	1475	- 1	12.427	5.8		21.828	1.0		. 78
ATOM	110	CA	ARG	1475	- 1	3.107	7.8	49	21.097	1.0		1.76
ATOM	111	CB	ARG	1475	-1	2.149	8.5	88	21.900	1.0	_	. 26
ATOM	112	CG	ARG	1475	-1	2.362	10.0	83 ;	21.743	1.0	_	.58
ATOM	113	CD	ARG		-1	2.178	10.5	36 :	20.342	1.0	_	.54
ATOM	114	NE	ARG	1475	-1	2.048	12.02	27 2	20.206	1.00		. 96
ATOM	116	CZ	ARG	1475		1.733	12.31	l7 ]	18.813	1.00		.07
ATOM	117	NH1	ARG	1475		0.503	12.50	)1 1	18.352	1.00		.07 .59
		-4417	AIRG	1475	- :	9.470	12.44		9.186	1.00		
CCCD In-										±.00	. 34	.89



					10	308	12.669	17.049	1.00	34.5 35.5	
MOTA	120	NH2	ARG	1475		2.173	8.261	23.371	1.00	37.0	
ATOM	123	С	ARG	1475		1.135	8.318	24.036	1.00	36.6	
MOTA	124	0	ARG	1475 1476	-13	3.356	7.958	23.889	1.00	37.0	
MOTA	125	N	ASP		-1	3.498	7.647	25.307	1.00	37.8	, , 17
MOTA	127	CA	ASP	1476		4.967	7.759	25.740	1.00	38.9	, , a 3
MOTA	128	CB	ASP	1476		5.851	6.704	25.115	1.00	43.	75
MOTA	129	CG	ASP	1476 1476		5.412	6.015	24.179	1.00	45.	
MOTA	130	OD1	ASP	1476		7.003	6.558	25.563	1.00	35.	
ATOM	131	OD2	ASP	1476		2.922	6.292	25.701	1.00		
MOTA	132	С	ASP	1476	-1	2.923	5.928	26.878	1.00		
MOTA	133	0	ASP	1477		2.478	5.527	24.711	1.00		
MOTA	134	N	ARG	1477	_	1.889	4.221	24.961	1.00		84
MOTA	136	CA	ARG			12.214	3.262	23.809	1.00 1.00		70
MOTA	137	CB	ARG			13.693	2.965	23.580			
MOTA	138	CG	ARG			14.366	2.365	24.809	1.00		
MOTA	139	CD	ARG			14.596	3.372	25.838	1.00		
MOTA		NE	ARG			14.845	3.102				.58
MOTA		CZ	ARC			14.906	1.846	27.542			.14
MOTA		NH1				15.024	4.102				.30
ATOM		NH2	AR			10.373	4.338				.32
MOTA		C	AR	<u>-</u>		-9.679	3.362	_			. 85
MOTA		0	LE			-9.856	5.544				.64
MOTA		N	LE	<u></u>		-8.426	5.73				.96
OTA		CA				-7.964	6.36				.36
OTA		CB				-6.498	6.29				71.
ATO!			_			-6.059	4.83				3.97
OTA						-6.335				00 31	7.60
ATO		_	L			-8.054				00 4	1.20
OTA		_	L			-8.366				00 3	6.52
OTA				AL 14	79	-7.442				00 3	5.59
ATO				AL 14	79	-7.008				00 3	5.92
ATC ATC				AL 14	79	-7.043				00 3	9.40
ATC ATC		_			79	-6.71				00 3	4.46
OTA TO		_			79	-8.40	_				5.36
ATC ATC		_			79	-5.57					32.50
AT(		_	v		179	-4.62	_		78 1.		37.77
TA	_		ı		180	-5.43			72 1		12.77
	OM 17	_			480	-4.13 -4.29	_		342 1		41.84
	OM 17	71 (			480	-4.99	•	69 25.4			42.45
	OM 17	72 (			480	-5.13		74 24.9	_		42.58
		73 (			480	-4.20	_	08 24.			43.09
					480	-3.2		233 28.			45.25
		75 (	_		480	-3.6		739 29.			45.47
			-		480	-1.9		816 28.		.00	46.82
			N		481	-1.9		889 29.		00	50.47
		79	CA		1481	0.2		617 29.	<del>-</del> ·	00	52.24
		.80	С		1481	0.2		638 28.		.00	53.41
		.81	0		1481	1.3	-	070 30.		1.00	53.64
		182	N		1482	2.6		627 30.	-	1.00	56.19
		184	CA		1482		=	776 30		1.00	57.19
		185	CB		1482			023 30		1.00	61.02 63.12
		186	CG	LYS	1482		•	831 31	.089	1.00	03.14
		187	CD	LYS	1482						

							120				
	ATOM	188	CE	LYS	1400						
	ATOM	189	NZ		1482	~ · · · .	94 6	.547 3	0.395	_	
	ATOM	193	C.	LYS	1482					1.00	
	ATOM	194		LYS	1482	3.29			0.899	1.00	63.38
	<b>.</b>		0	LYS	1482	3.29			8.604	1.00	56.56
		195	N	PRO	1483	3.85			7.791	1.00	55.03
		196	CD	PRO	1483		- •	983 28	3.323	1.00	58.31
		197	CA	PRO	1483	3.85		191 29	.167	1.00	
2	MOTA	198	CB	PRO		4.46		254 27	.020		56.98
Į	ATOM :	199	CG	PRO	1483	4.91	12.		.155	1.00	59.52
7	ATOM 2	200	C		1483	3.92 <sup>.</sup>	7 13.:			1.00	58.75
		201		PRO	1483	5.673	10.		.141	1.00	58.79
			0	PRO	1483	6.509			. 834	1.00	61.17
	_		N	LEU	1484	5.728			.731	1.00	61.31
			CA	LEU	1484	5.720			. 702	1.00	64.31
	TOM 2	05	CB	LEU	1484	6.838	8.7	38 25	408	1.00	
	TOM 2	06		LEU		6.349		12 24	640		67.77
	TOM 2	~ _	~~-		1484	5.415	6.5		386	1.00	67.66
A	TOM 20				1484	4.943	5.4			1.00	69.00
			~		1484	6.126	5.9		445	1.00	66.76
		`		EU	1484	7.934			604	1.00	67.77
			_	EU :	1484	9.117	9.4			1.00	70.82
		_	1 G		1485		9.13				71.82
	'OM 21	3 0	'A G		1485	7.534	10.35	7 23.		_	
AT		4 C			485	8.492	11.07	7 22.			73.28
AT	OM 21		_			7.819	11.75	4 21.			74.53
AT	OM 21		_		485	6.635	12.09	0 21.8			75. <b>1</b> 9
ATO	OM 21				491	4.406	14.27	_		00	75.61
ATO		_	_		491	4.042	13.87			.00	50.72
ATC			B GI	N 1	491	3.033			94 1		17.33
ATC			GI	N 1	491	3.486	14.86	. •			6.67
		_	GI		491		12.44	9 20.0	73 1		6.66
ATO			VA		192	2.581	12.074	19.3	~ ~		
ATO		CA			192	4.072	11.650	20.9		-	5.20
ATO		CB				3.646	10.274	21.18			5.41
ATO					92	4.680	9.244			00 4	3.83
ATO	M 227	CG			92	4.138	7.849			00 4	1.60
ATO					92	5.007	9.445			00 4	1.35
ATON		C	VAI		92	3.458	10.084			00 42	2.72
ATOM		0	IAV	14	92	4.335	10.084				.45
ATOM		N	VAI	14:	93	2.309	10.437	23.48			.86
		CA	VAI			2.509	9.548	23.07	0 1.		.67
ATOM		CB	VAL			2.029	9.321	24.47			
ATOM	~	CG1				0.884	10.242	25.01			.05
ATOM	235	CG2		_		1.177	11.693	24.72	_		.64
ATOM		C	*			0.459	9.844	24.42	• •		. 40
ATOM		ō	VAL	149		1.626	7.880	24.92			.36
ATOM			VAL	149	3	1.129	7.212	24.704			.09
ATOM		N	LEU	149	4	1.927	7 274	23.796		0 39	
ATOM	240	CA	LEU	149	4	1.535	7.374	25.890	1.0	0 37.	
	241	CB	LEU	149	4	2.353	6.036	26.250	1.0		
ATOM	242	CG	LEU	149		2.359	5.542	27.440	1.0	•	
ATOM	243	CD1	LEU			2.036	4.161	28.007	1.0		
ATOM	244	CD2		1494		2.123	3.085	26.931			
ATOM	245	C	LEU	1494	-	. 998	3.860		1.0		
ATOM	246		LEU	1494	l 0	.077	6.236	29.143	1.0		99
ATOM		0	LEU	1494	-0	.311		26.648	1.00	33.	
ATOM	247	N	ALA	1495		.740	7.318	27.097	1.00	32.	
	249	CA	ALA	1495	_	.147	5.219	26.435	1.00		
ATOM	250	CB	ALA	1495	_		5.292	26.773	1.00		
ATOM	251	С	ALA	1495			5.937	25.637	1.00		
				<b>477</b> 5	-2		_	27.025			
SSSD/55	145, vn1								1.00	29.9	7
	-: 701										

MOTA 252 2.909 0 ALA 1495 -1.944 26.840 1.00 28.15 **ATOM** 253 Ν GLU 1496 -3.898 3.813 27.488 1.00 30.37 **ATOM** 255 -CA GLU 1496 -4.537 2.536 27.745 1.00 31.47 **ATOM** 256 CB GLU 1496 -4.862 2.392 29.223 1.00 32.48 CG **ATOM** 257 GLU 1496 -3.627 2.239 30.093 1.00 37.81 MOTA 258 CD GLU 1496 -3.938 2.426 31.565 1.00 41.09 **ATOM** 259 OE1 GLU 1496 3.548 -4.328 31.944 1.00 41.53 ATOM 260 OE2 GLU 1496 -3.797 1.453 32.341 1.00 44.12 ATOM 261 C GLU 1496 -5.806 2.524 26.916 1.00 32.72 **ATOM** 262 0 GLU 1496 -6.586 3.478 26.954 1.00 33.91 **ATOM** 263 N ALA 1497 -5.953 1.494 26.094 1.00 31.06 ATOM 265 CA ALA 1497 -7.117 1.353 25.239 1.00 32.33 ATOM 266 CB ALA 1497 -6.691 0.879 23.859 1.00 29.56 MOTA 267 C ALA 1497 -8.056 0.343 25.885 1.00 32.26 MOTA 268 0 ALA 1497 -7.648 26.197 -0.773 1.00 33.55 MOTA 269 N ILE 1498 -9.286 0.759 26.160 1.00 32.99 ATOM 271 CA ILE 1498 -10.276 -0.126 26.766 1.00 34.00 MOTA 272 CB ILE 1498 27.592 -11.329 0.668 1.00 34.69 MOTA 273 CG2 ILE 1498 -12.341 -0.288 28.240 1.00 34.24 **ATOM** 274 CG1 ILE 1498 -10.647 1.496 28.686 1.00 33.56 **ATOM** 275 CD1 ILE 1498 -11.543 2.572 29.258 1.00 31.25 ATOM 276 C ILE 1498 -10.994 -0.830 25.624 1.00 35.71 **ATOM** 277 0 ILE 1498 -11.618 -0.181 24.786 1.00 34.88 ATOM 278 GLY N 1499 -10.890 -2.147 25.573 1.00 40.43 **ATOM** 280 CA GLY 1499 -11.553 -2.884 24.516 1.00 47.63 ATOM 281 С GLY 1499 -10.670 -3.233 23.330 1.00 53.08 ATOM 282 0 GLY 1499 -9.934 -4.226 23.380 1.00 54.97 **ATOM** 283 N LEU 1500 -10.713 -2.394 22.294 1.00 54.18 MOTA 285 CA LEU 1500 -9.957 -2.603 21.055 1.00 55.26 MOTA 286 CB LEU 1500 -8.444 -2.726 21.305 1.00 55.39 MOTA 287 CG LEU 1500 -7.562 -1.472 21.241 1.00 54.27 MOTA 288 CD1 LEU 1500 -6.110 -1.891 21.367 1.00 52.89 MOTA 289 CD2 LEU 1500 -7.768 -0.711 19.935 1.00 50.91 MOTA 290 С LEU 1500 -10.453 -3.830 20.288 1.00 55.39 MOTA 291 О LEU 1500 -10.376 -4.963 20.774 1.00 56.23 **ATOM** 292 N PRO 1505 -13.315 -5.836 25.394 1.00 53.03 ATOM 293 CD PRO 1505 -13.945 -7.148 25.167 1.00 55.12 ATOM 294 CA PRO 1505 -14.306 -4.848 25.846 1.00 50.62 **ATOM** 295 CB PRO 1505 -15.635 -5.607 25.715 1.00 50.09 MOTA 296 CG PRO 1505 -15.241 -7.031 25.950 1.00 52.18 **ATOM** 297 C PRO 1505 -14.039 -4.348 27.273 1.00 46.35 MOTA 298 О PRO 1505 -14.065 -3.143 27.524 1.00 45.82 MOTA 299 N ASN 1506 -13.711 -5.261 28.181 1.00 42.76 MOTA 301 CA ASN 1506 -13.433 -4.892 29.566 1.00 45.29 MOTA 302 CB ASN 1506 -14.283 -5.728 30.529 1.00 45.92 MOTA 303 CG ASN 1506 -15.752 -5.395 30.441 1.00 46.17 **ATOM** 304 OD1 ASN 1506 -16.132 -4.232 30.390 1.00 48.57 ATOM 305 ND2 ASN 1506 -16.589 -6.418 30.406 1.00 48.63 MOTA 308 С ASN 1506 -11.954 -5.008 29.939 1.00 45.33 MOTA 309 ASN 0 1506 -11.597 -5.084 31.121 1.00 44.53 MOTA 310 N ARG 1507 -11.100 -5.010 28.924 1.00 45.63 MOTA 312 CA ARG 1507 -9.660 -5.122 29.117 1.00 45.57 ATOM 313 CB ARG 1507 -9.131 -6.354 28.375 1.00 53.33

SSSD/55145. v01

314

CG

ARG

1507

-9.407

-7.685

29.043

1.00

61.39

MOTA

		315	CD	ARG	1507	-8.33	_				
		16	NE	ARG	1507		- •		063	1.00	67.74
			CZ	ARG	1507	0.52		-	585	1.00	74.64
			NH1	ARG	1507	, , , , ,			701	1.00	80.01
			NH2	ARG	1507	-8.268				1.00	80.04
			C,	ARG	1507	-8.964	-			1.00	83.41
			0	ARG	1507	-9.370				1.00	40.94
			7 7	/AL	1508	-7.956				1.00	37.60
			r AS	/AL	1508	-7.190				1.00	39.33
	OM 33		CB (	'AL	1508	-6.854				1.00	37.26
	OM 33	-	G1 V	'AL	1508	-8.124	-1.2	_		1.00	36.25
TA TA				AL	1508	-5.903	-0.7	_		1.00	39.63
AT			•	AL	1508	-5.898	-1.79 -2.81			1.00	36.92
ATO		_	•	AL	1508	-5.387	-3.85	_		1.00	34.38
ATO			-	HR	1509	-5.406	-2.14			1.00	32.85
ATO		_		HR	1509	-4.174	-2.52			1.00	30.47
ATC		_			1509	-4.455	-2.95			1.00	31.65
ATO					1509	-5.426	-4.01			1.00	34.13
ATO			32 TI	IR	1509	-3.184	-3.45			1.00	40.74
ATO			TF	IR .	1509	-3.270	-1.29				31.06
ATO			TH		1509	-3.716	-0.219	_		1.00	28.38
ATO	~		LY	_	1510	-2.023	-1.442		_		27.78
ATO					L510	-1.101	-0.312				29.48
ATO	,				L510	0.172	-0.558	-0.05			30.54
ATON					.510	~0.037	-0.600		_		27.88
ATON		CD CE		_	510	1.284	-0.759			.00	33.91
ATOM		NZ	LY	_	510	1.145	-1.674			.00 4	10.30
ATOM	_	C	LY		510	0.338	-1.096			.00 4	6.24
ATOM		0	LYS		510	-0.757	-0.166	25.36			9.09
ATOM		N	LYS	_	510	-0.402	-1.142	24.704			8.64
ATOM		CA	VAI		511	~0.902	1.048	24.856			8.76
ATOM		CB	IAV IAV		511	-0.627	1.347	23.463			9.34
ATOM		CG1			511	-1.951	1.457	22.658			9.79
ATOM	362	CG2			511 511	-2.681	0.111	22.657			7.14 4.56
ATOM	<b>•36</b> 3	C	VAL		511	-2.837	2.561	23.243	1.		2.15
ATOM	364	0	VAL		11	0.123	2.672	23.361	1.		9.83
ATOM	365	N	ALA		12	0.213	3.413	24.338	1.		3.14
MOTA	367	CA	ALA		12	0.705	2.939	22.196	1.0		7.86
MOTA	368	CB	ALA		12	1.405	4.192	21.962	1.(		.55
ATOM	369	C	ALA	15		2.743 0.500	3.935	21.297	1.0		.69
ATOM	370	0	ALA	15		-0.061	5.009	21.057	1.0		. 25
ATOM	371	N	VAL	15		0.340	4.483	20.107	1.0		.18
ATOM	<b>37</b> 3	CA	VAL	15:		0.520	6.289	21.360	1.0		. 63
ATOM	374	CB	VAL	153		1.704	7.165	20.573	1.0		.66
ATOM	375	CG1	VAL	151		2.609	7.713	21.422	1.0		.47
MOTA	376	CG2	VAL	151		2.509	8.585	20.574	1.0		. 29
ATOM	377	C	VAL	151		0.238	6.559	22.031	1.0	0 32.	
ATOM	378	0	VAL	151		0.792	8.334	19.938	1.0		
ATOM	379	N	LYS	151		0.792	9.185	20.635	1.0		
ATOM	381	CA	LYS	151		0.207	8.367	18.605	1.00	36.	
ATOM	382	CB	LYS	151		1.349	9.390	17.789	1.00	36.	
ATOM	383	CG	LYS	151		2.250		16.489	1.00	36.	
MOTA	384	CD	LYS	151		2.559		16.697	1.00	39.	
SSSD/55	•						6.854	15.390	1.00	45.	
3331 J/55'	115										



ATOM	385	CE	LYS	1514	3.080	7.815	14.331	1.00	50.70
ATOM	386	NZ	LYS	1514	4.212	8.685	14.798	1.00	51.41
ATOM	390	С	LYS	1514	-0.121	10.496	17.459	1.00	36.75
ATOM	391	0	LYS	1514	-1.228	10.234	16.978	1.00	35.42
MOTA	392	N	MET	1515	0.294	11.731	17.700	1.00	38.12
MOTA	394	CA	MET	1515	-0.545	12.882	17.432	1.00	41.90
ATOM	395	CB	MET	1515	-1.371	13.238	18.668	1.00	43.08
ATOM	396	CG	MET	1515	-0.536	13.601	19.880	1.00	45.01
ATOM	397	SD	MET	1515	-1.561	13.784	21.324	1.00	46.03
ATOM	398	CE	MET	1515	-1.675	12.072	21.885	1.00	44.02
ATOM	399	С	MET	1515	0.314	14.065	17.021	1.00	44.65
MOTA	400	0	MET	1515	1.543	14.013	17.094	1.00	45.64
MOTA	401	N	LEU	1516	-0.347	15.123	16.568	1.00	47.08
ATOM	403	CA	LEU	1516	0.329	16.337	16.134	1.00	48.08
MOTA	. 404	CB	LEU	1516	~0.500	17.033	15.054	1.00	45.50
ATOM	405	CG	LEU	1516	-0.764	16.265	13.764	1.00	43.22
MOTA	406	CD1	LEU	1516	-1.783	17.014	12.946	1.00	40.32
ATOM	407	CD2	LEU	1516	0.540	16.072	12.991	1.00	43.78
ATOM	408	С	LEU	1516	0.516	17.302	17.297	1.00	51.27
ATOM	409	0	LEU	1516	-0.214	17.249	18.291	1.00	50.37
ATOM	410	N	LYS	1517	1.491	18.191	17.157	1.00	55.47
MOTA	412	CA	LYS	1517	1.757	19.207	18.168	1.00	59.10
MOTA	413	CB	LYS	1517	3.203	19.702	18.068	1.00	61.61
ATOM	414	CG	LYS	1517	4.251	18.669	18.462	1.00	64.82
ATOM	415	CD	LYS	1517	5.635	19.109	18.018	1.00	67.42
MOTA	416	CE	LYS	1517	6.696	18.102	18.432	1.00	71.76
MOTA	417	NZ	LYS	1517	8.021	18.411	17.812	1.00	73.57
MOTA	421	С	LYS	1517	0.794	20.365	17.920	1.00	59.91
ATOM	422	0	LYS	1517	0.187	20.456	16.852	1.00	59.88
ATOM	423	N	SER	1518	0.686	21.267	18.886	1.00	61.85
MOTA	425	CA	SER	1518	-0.216	22.409	18.760	1.00	63.70
ATOM	426	CB	SER	1518	-0.158	23.274	20.024	1.00	64.21
ATOM	427	С	SER	1518	0.079	23.263	17.529	1.00	64.37
MOTA	428	0	SER	1518	-0.841	23.757	16.875	1.00	66.16
ATOM	429	N	ASP	1519	1.359	23.410	17.202	1.00	64.15
MOTA	431	CA	ASP	1519	1.767	24.217	16.054	1.00	64.55
ATOM	432	СВ	ASP	1519	3.109	24.897	16.343	1.00	65.84
ATOM	433	C	ASP	1519	1.858	23.441	14.742	1.00	63.95
ATOM	434	0	ASP	1519	2.432	23.931	13.769	1.00	64.95
ATOM	435	N	ALA	1520	1.303	22.232	14.719	1.00	62.57
ATOM	437	CA	ALA	1520	1.329	21.398	13.521	1.00	60.34
ATOM	438	CB	ALA	1520	0.704	20.039	13.810	1.00	60.53
ATOM	439	C	ALA	1520	0.616	22.062	12.353	1.00	58.21
ATOM	440	0	ALA	1520	-0.464	22.631	12.506	1.00	58.32
ATOM	441	N	THR	1521	1.241	22.001	11.186	1.00	55.96
ATOM	443	CA	THR	1521	0.673	22.582	9.981	1.00	54.98
ATOM	444	CB	THR	1521	1.783	23.013	9.031	1.00	53.84
ATOM	445	OG1	THR	1521	2.554	21.862	8.659	1.00	55.84
ATOM	447	CG2	THR	1521	2.693	24.026	9.703	1.00	55.01
ATOM	448	C	THR	1521	-0.184	21.545	9.261	1.00	54.25
ATOM	449	0	THR	1521	-0.190	20.371	9.629	1.00	54.74
ATOM	450	N	GLU	1522	-0.877	21.974	8.212	1.00	53.32
ATOM	452	CA	GLU	1522	-1.702	21.066	7.423	1.00	52.64
ATOM	453	CB	GLU	1522	-2.472	21.829	6.339	1.00	53.55

ATO	OM 454	· C	GL	.TT 1522					
ATO		_	GL						51.95
ATO		_	LY					4 1.00	53.28
ATC								4 1.00	
ATC				_					
ATO					2.730		5.620	1.00	
ATO	•				3.889				
ATO					3.487	18.388	4.016		
ATO			LY	_	4.688	17.635			
		NZ	LYS	5 1523	4.271	16.629			
ATO		C	LYS	1523	1.699	18.391			
ATO		0	LYS	1523	1.747	17.202			
ATO	_	N	ASI		1.857	18.828			
ATO		CA	ASF		2.114	17.915	8.249		42.71
OTA	M 472	CB	ASF		2.313		9.351		42.11
ATO		CG	ASP		3.623	18.701			44.94
ATON	474	OD1			3.692	19.490	10.673		48.90
MOTA	475	OD2				20.512	11.392		51.88
ATOM	476	С	ASP		4.590	19.084	9. <b>99</b> 0	1.00	50.06
ATOM	1 477	0	ASP		0.956	16.931	9.481	1.00	39.85
ATOM	1 478	N	LEU		1.164	15.738	9.748	1.00	39.01
ATOM		CA	LEU		-0.261	17.438	9.296	1.00	38.32
ATOM		CB	LEU		-1.461	16.610	9.355	1.00	36.16
ATOM		CG			-2.720	17.470	9.200	1.00	35.13
ATOM		CD1	LEU		-4.081	16.760	9.186	1.00	34.70
ATOM		CD2	LEU	1525	-4.184	15.668	10.252	1.00	36.15
ATOM			LEU	1525	-5.162	17. <b>78</b> 9	9.395	1.00	32.96
ATOM		С	LEU	1525	-1.406	15.560	8.254	1.00	34.31
ATOM	_	0	LEU	1525	-1.575	14.377	8.518	1.00	33.34
ATOM		N	SER	1526	-1.136	16.005	7.030	1.00	36.40
ATOM		CA	SER	1526	-1.039	15.128	5.865	1.00	37.16
	490	CB	SER	1526	~0.669	15.931	4.618	1.00	
ATOM ATOM	491	OG	SER	1526	-1.736	16.779	4.245	1.00	38.84
	493	C	SER	1526	-0.021	14.016	6.044	1.00	49.61
ATOM	494	0	SER	1526	-0.273	12.873	5.670	1.00	35.90
ATOM	495	N	ASP	1527	1.142	14.349	6.591		36.68
ATOM	497	CA	ASP	1527	2.177	13.342	6.796	1.00	35.89
ATOM	498	CB	ASP	1527	3.497	13.998	7.201	1.00	35.25
ATOM	499	CG	ASP	1527	4.100	14.850		1.00	35.58
ATOM	500	OD1	ASP	1527	3.750	14.653	6.081	1.00	37.19
ATOM	501	OD2	ASP	1527	4.932	15.726	4.895	1.00	37.38
ATOM	502	С	ASP	1527	1.749	12.274	6.395	1.00	42.93
ATOM	503	0	ASP	1527	2.000	11.090	7.799	1.00	31.77
ATOM	504	N	LEU	1528	1.055	12.684	7.594	1.00	30.58
ATOM	506	CA	LEU	1528	0.581		8.853	1.00	31.80
ATOM	507	CB	LEU	1528	-0.002	11.730	9.857	1.00	33.53
ATOM	508	CG	LEU	1528			11.076		32.20
ATOM	509	CD1	LEU	1528	-0.440		12.275	1.00	32.63
ATOM	510	CD2	LEU	1528	0.705		12.709	1.00	33.09
ATOM	511	C			-0.891		13.426	1.00	31.52
ATOM	512	0	LEU	1528	-0.468	10.792	9.235		32.89
ATOM	513		LEU	1528	-0.494	9.589	9.521		32.39
ATOM	515	N	ILE	1529	-1.336	11.357	8.393		33.72
ATOM	516	CA	ILE	1529	-2.376	10.591			30.48
MOTA		CB	ILE	1529	-3.336	11.505	_		28.85
ATOM	517	CG2	ILE	1529	-4.229	10.662			28.54
AT ON	518	CG1	ILE	1529	-4.200	12.344			29.5 <u>2</u>
SSSD/FF							••		~J.JZ



MOTA 519 CD1 ILE 1529 -5.143 13.308 7.133 1.00 32.07 MOTA 520 С ILE 1529 -1.698 9.608 6.768 1.00 31.50 MOTA 521 0 ILE 1529 -2.009 8.419 6.780 1.00 30.75 ATOM 522 N SER 1530 -0.749 10.100 5.974 1.00 33.28 **ATOM** 524 CA SER 1530 -0.011 9.250 5.038 1.00 32.48 **ATOM** 525 CB SER 1530 1.114 10.042 4.368 1.00 37.20 MOTA 526 OG SER 1530 0.604 11.218 3.766 1.00 49.93 ATOM 528 C SER 1530 0.583 8.045 1.00 5.756 29.05 MOTA 529 0 SER 1530 0.397 6.909 5.316 1.00 28.66 **ATOM** 530 N GLU 1531 1.259 8.290 6.878 1.00 28.21 MOTA 532 CA GLU 1531 1.880 7.207 7.631 1.00 27.30 MOTA 533 CB GLU 1531 2.656 7.733 8.839 1.00 28.90 MOTA 534 CG GLU 1531 3.271 6.609 9.672 1.00 27.17 MOTA 535 CDGLU 1531 4.047 7.081 10.886 1.00 30.07 MOTA 536 OE1 GLU 1531 4.779 6.244 11.448 1.00 34.78 MOTA 537 OE2 GLU 1531 3.931 8.256 11.291 1.00 31.96 ATOM 538 С GLU 1531 0.870 6.162 8.072 1.00 27.73 MOTA 539 0 GLU 1531 1.160 4.961 8.028 1.00 28.72 ATOM 540 N MET 1532 -0.286 6.621 8.555 1.00 29.78 ATOM 542 MET CA 1532 -1.373 1.00 5.734 8.990 28.79 ATOM 543 CB MET 1532 -2.501 6.553 9.646 1.00 28.90 ATOM 544 CG MET 1532 -3.763 5.741 9.993 1.00 29.73 **ATOM** 545 SD MET 1532 -5.089 6.693 10.765 1.00 30.19 MOTA 546 CE MET 1532 -5.455 7.870 9.494 1.00 26.70 MOTA 1532 547 С MET -1.935 4.937 7.796 1.00 28.34 ATOM 548 0 MET 1532 -2.166 3.730 7.893 1.00 26.62 ATOM 549 N GLU 1533 -2.165 5.624 6.678 1.00 28.85 MOTA 551 CA GLU 1533 -2.684 4.984 5.467 1.00 28.24 MOTA 552 CB GLU 1533 -2.936 6.027 4.384 1.00 25.42 ATOM 553 CG GLU 1533 -4.099 6.956 1.00 4.719 30.05 MOTA 554 CD GLU 1533 -5.393 6.201 5.021 1.00 29.47 MOTA 555 OE1 GLU 1533 -5.794 5.336 4.211 1.00 29.01 MOTA 556 OE2 GLU 1533 -6.011 6.472 6.073 1.00 33.98 **ATOM** 557 C GLU 1533 -1.694 3.944 4.968 1.00 28.01 MOTA 558 0 GLU 1533 -2.072 2.845 4.573 1.00 27.39 **ATOM** 559 N MET 1534 -0.416 4.293 5.036 1.00 29.06 ATOM 561 CA MET 1534 0.662 3.413 4.621 1.00 29.74 **ATOM** 562 CB MET 1534 1.992 4.155 4.755 1.00 33.16 MOTA 563 CG MET 1534 3.198 3.270 4.682 1.00 42.88 ATOM 564 SD MET 1534 3.805 3.127 3.042 1.00 50.20 ATOM 565 CE MET 1534 5.137 4.169 3.159 1.00 42.64 **ATOM** 566 С MET 1534 0.641 2.156 5.493 1.00 26.90 **ATOM** 567 0 MET 1534 0.755 1.038 4.990 1.00 27.05 **ATOM** 568 N MET 1535 0.512 2.348 6.803 1.00 25.42 MOTA 570 CA MET 1535 0.437 1.233 7.737 1.00 25.88 **ATOM** 571 CB MET 1535 0.325 1.741 9.181 1.00 27.63 **ATOM** 572 CG MET 1535 1.607 2.391 9.737 1.00 27.26 MOTA 573 SD MET 1535 1.584 2.561 11.564 1.00 29.49 ATOM 574 CE MET 1535 1.294 4.255 11.699 1.00 28.22 MOTA 575 MET C 1535 -0.754 0.324 7.396 1.00 26.28 MOTA 576 0 MET 1535 -0.645 -0.908 7.469 1.00 25.93 **ATOM** 577 N LYS 1536 -1.890 0.928 7.032 1.00 27.19 MOTA 579 CA LYS 1536 -3.087 0.162 6.647 1.00 27.20 MOTA 580 CB LYS 1536 -4.257 1.088 6.310 1.00 25.29

							1	.26						
	ATOM	581	CG	LYS	1524									
	ATOM	582	CD	LYS	1536		897	1.	770	7.49	. 1		_	
i	ATOM	583	CE		1536		884		820	7.01		1.00	23.	
2	MOTA	584	NZ	LYS	1536		460		588	8.17		.00	22.	
		588	C	LYS	1536		484		541		_	00	22.	
		589		LYS	1536	-2.			699	7.71		.00	23.4	<b>4</b> O
			0	LYS	1536	~3.0				5.42		.00	24.5	
		590	N	MET	1537	-2.]	100	-1.		5.40		.00	26.6	
		592	CA	MET	1537	-1 0	143	-0.		4.41		.00	27.1	
		593	CB	MET	1537	-1.8	43	-0.8		3.194		.00		
		94	<b>-</b>	MET	1537	-1.2	69	0.]	47	2.147	_	.00	28.0	
	TOM 5	95	~-	MET		-2.2	65	1.1	.64	1.591			30.3	
A'	TOM 5	96	~~	MET	1537	0.0		0.4	44	0.727		00	36.3	
A:	rom 5	97	~		1537	-2.9		-0.0		0.793		00	42.1	
A7				/ET	1537	-0.8	57	-1.9				00	36.22	2
		_		1ET	1537	-1.06	50	-3.0	-	3.447			26.98	3
				LE	1538	0.18			_	2.963	1.	00	25.34	
				LE	1538	1.23		-1.6	_	4.229	1.	00	27.69	
			CB I	LE	1538	2.45		-2.6	74	4.535	1.0		25.39	
	OM 60		CG2 I	LE	1538			-2.00	)6 9	5.255	1.0		24.42	
AT		)4 (	~~~		1538	3.42		-3.05	51 9	5.811	1.0			
AT						3.22		-1.13	1 4	1.269	1.0		25.28	
ATO	OM 60	6 c			1538	4.37		-0.37		.901			23.88	
ATO					1538	0.76		~3.92		.292	1.0		27.19	
ATO	OM 60	_			L538	1.24	2	-5.03		.035	1.0		25.59	
ATO			٠.	_	1539	-0.19	3	-3.76			1.0		6.11	
ATC	DM 61:				.539	-0.661		-4.94		-208	1.0		6.13	
ATO		. •	-	_	539	0.19]				. 934	1.0	0 2	5.25	
ATO				Y 1	539	1.214		-5.28		.149	1.0	_	6.77	
ATO	_		LY	S 1	540	-0.204		-4.63	-	.414	1.00		5.42	
			J LY		540			-6.327		862	1.00		5.62	
ATO			B LY		540	0.467		-6.716		092	1.00		5.38	
ATO		CG		_	540	-0.552		7.283	11.	084	1.00			
ATO		CD			540	-1.573	-	6.303		550	1.00	_	7.15	
ATON						-2.528	-	6.943					1.23	
ATOM	<b>1</b> 620	NZ			540	-3.559		5.927			1.00		.69	
ATOM	1 624	C			40	-2.956		4.800	13.	_	1.00		.08	
ATOM			LYS		40	1.609		7.705			1.00	44	.05	
ATOM		0	LYS		40	1.627		8.600	10.		1.00	24	.37	
ATOM		N	HIS	15	41	2.545		7.538		181	1.00	26	.12	
ATOM		CA	HIS	15	41	3.666		, , , , , ,	10.9		1.00		.41	
ATOM		CB	HIS	15		4.772	- (	8.440	11.0		1.00		. 41	
ATOM		CG	HIS	15		5.798	- 8	3.228	10.0		00		. 88	
	631	CD2	HIS	15			- 5	3.320	10.0		.00	22		
ATOM	632	ND1		154		5.823	~10	.522	9.4		.00	21.		
MOTA	634	CE1		154		6.939	- 9	.268	10.8		.00			
ATOM	635	NE2				7.619	-10	.389	10.6	<b>_</b>	.00	22.		
ATOM	637	C		154		6.966	-11	.167	9.8			24.		
ATOM	638	ō	HIS	154		4.234		.328	12.4		.00	27.	00	
ATOM	639		HIS	154	1	4.364		.239	12.4		.00	25.	47	
ATOM		N	LYS	154	2 .	4.560	- 0	.476	13.0		00	26.	77	
ATOM	641	CA	LYS	154		5.127	ء ۔	-3/0	13.06		.00	26.	38	
ATOM	642	CB	LYS	154		5.515		. 552	14.40		00	30.0		
	643	CG	LYS	154	-		-11.	.003	14.69	2 1.	00	31.3		
MOTA	644	CD	LYS	1542		.061		252	16.07		00			
ATOM	645	CE	LYS		_	.289	-12.	735	16.29		00	42.7		
ATOM	646	NZ		1542		.041	-13.	374	15.11			50.8		
ATOM	650	C	LYS	1542		.511	-14.		15.42		00	56.7		
ATOM	651		LYS	1542		.342	-8.					61.2		
•	1	0	LYS	1542		.519	-8.		14.62	•		27.6		
SSSD/55	145 . 0-						٠.		15.71	1 1.		26.8		
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ATOM	652	N	ASN	1543	7.146	-8.445	13.585	1.00	27.20
MOTA	654	CA	ASN	1543	8.354	-7.642	13.735	1.00	25.50
MOTA	655	CB	ASN	1543	9.578	-8.431	13.260	1.00	25.59
MOTA	656	CG	ASN	1543	9.712	-9.767	13.974	1.00	22.64
ATOM	657	OD1	ASN	1543	9.522	-10.821	13.371	1.00	26.76
MOTA	658	ND2	ASN	1543	9.970	-9.727	15.273	1.00	25.56
ATOM	661	С	ASN	1543	8.374	-6.213	13.226	1.00	25.48
ATOM	662	0	ASN	1543	9.417	-5.692	12.842	1.00	24.58
MOTA	663	N	ILE	1544	7.209	-5.575	13.244	1.00	24.60
ATOM	665	CA	ILE	1544	7.065	-4.177	12.868	1.00	22.32
MOTA	666	CB	ILE	1544	6.524	-3.972	11.409	1.00	25.82
MOTA	667	CG2	ILE	1544	7.401	-4.720	10.403	1.00	24.24
ATOM	668	CG1	ILE	1544	5.057	-4.411	11.279	1.00	26.04
MOTA	669	CD1	ILE	1544	4.446	-4.121	9.901	1.00	23.20
MOTA	670	С	ILE	1544	6.075	-3.598	13.881	1.00	22.37
ATOM	671	0	ILE	1544	5.364	-4.345	14.559	1.00	21.68
ATOM	672	N	ILE	1545	6.111	-2.290	14.076	1.00	23.72
ATOM	674	CA	ILE	1545	5.169	-1.650	14.989	1.00	25.92
ATOM	675	CB	ILE	1545	5.602	-0.199	15.364	1.00	27.24
ATOM	676	CG2	ILE	1545	4.452	0.554	16.035	1.00	22.76
ATOM	677	CG1	ILE	1545	6.839	-0.219	16.285	1.00	25.57
ATOM	678	CD1	ILE	1545	6.591	-0.797	17.686	1.00	24.66
ATOM	679	C	ILE	1545	3.877	-1.612	14.179	1.00	26.03
ATOM	680	0	ILE	1545	3.823	-0.988	13.122	1.00	25.70
ATOM	681	N	ASN	1546	2.849	-2.293	14.669	1.00	24.79
ATOM	683	CA	ASN	1546	1.577	-2.354	13.956	1.00	25.51
ATOM	684	CB	ASN	1546	0.922	-3.727	14.137	1.00	25.17
ATOM	685	CG	ASN	1546	1.730	-4.839	13.539	1.00	21.67
ATOM	686	OD1	ASN	1546	1.856	-4.947	12.329	1.00	24.29
ATOM	687	ND2	ASN	1546	2.278	-5.686	14.384	1.00	22.24
MOTA	690	C	ASN	1546	0.578	-1.276	14.349	1.00	26.85
ATOM	691	0	ASN	1546	0.630	-0.724	15.453	1.00	28.67
MOTA	692	N	LEU	1547	-0.301	-0.956	13.407	1.00	27.70
ATOM	694	CA	LEU	1547	-1.357	0.019	13.622	1.00	27.64
ATOM	<b>69</b> 5	CB	LEU	1547	-1.945	0.481	12.284	1.00	24.87
ATOM	696	CG	LEU	1547	-3.173	1.400	12.337	1.00	23.25
MOTA	697	CD1	LEU	1547	-2.790	2.763	12.929	1.00	23.76
MOTA	698	CD2	LEU	1547	-3.757	1.569	10.923	1.00	23.47
ATOM	699	С	LEU	1547	-2.415	-0.771	14.396	1.00	27.27
ATOM	700	0	LEU	1547	-2.663	-1.952	14.103	1.00	25.27
MOTA	701	N	LEU	1548	-3.000	-0.130	15.400	1.00	27.94
MOTA	703	CA	LEU	1548	- <b>4</b> .017	-0.770	16.223	1.00	26.98
MOTA	704	CB	LEU	1548	-3.623	-0.735	17.708	1.00	24.65
MOTA	705	CG	LEU	1548	-2.327	-1.450	18.108	1.00	25.38
MOTA	706	CD1	LEU	1548	-2.189	-1.428	19.613	1.00	25.73
MOTA	707	CD2	LEU	1548	-2.337	-2.886	17.621	1.00	23.92
ATOM	708	С	LEU	1548	-5.369	-0.113	16.042	1.00	26.65
MOTA	709	0	LEU	1548	-6.392	-0.752	16.238	1.00	27.11
ATOM	710	N	GLY	1549	-5.378	1.163	15.684	1.00	25.04
ATOM	712	CA	GLY	1549	-6.643	1.855	15.516	1.00	25.47
ATOM	713	C	GLY	1549	-6.417	3.336	15.367	1.00	26.23
ATOM	714	Ō	GLY	1549	-5.267	3.781	15.287	1.00	28.41
MOTA	715	N	ALA	1550	-7.501	4.104	15.349	1.00	25.49
MOTA	717	CA	ALA	1550	-7.408	5.550	15.198	1.00	24.81
		- · -							- · · · · ·

							120						
	ATOM	718	СВ	ALA	1550	_							
		719	C		1550 1550			5.913	13.7	24 1	1.00	<b>.</b>	
		720	0		1550	-8.6		6.271	15.69		.00	21.7	
		721	N	<b>~</b>	1551	-9.7		5.702	15.72		.00	25.5	
		723	CA			-8.4		7.527	16.08		.00	24.0	
		724	CB	-	551	-9.4		8.438	16.51		.00	24.9	
	TOM ;	725	SG		551	-9.2		8.932	17.94		.00	26.80	
A	TOM 7	26	C		551	-9.3	33	7.655	19.22			26.32	
A'	TOM 7	27	0	_	551	-9.34	11	9.585	15.50		. 00 . 00	32.31	
	TOM 7	28	N	_	551	-8.36	51 1	0.338	15.53			28.31	
					552	-10.26	1	9.660	14.54		00	28.42	
A	COM 7	~ -			552	-10.19	8 10	0.671	13.498		00	28.38	
					552	-10.15	9 9	9.977	12.095		00	31.26	
ΑT	'OM 7:			_	552	-11.40	6 9	9.309	11.836			30.07	
AT	'OM 73		_		52	-9.04	4 B	.945	12.053			29.64	
AT	OM 73				52	-11.35	5 11	.662	13.509			28.65	
AT		7 N				-11.29	5 12	.722	12.874			33.31	
AT	OM 73	_				-12.420	) 11	.309	14.214	1.0		31.94	
ATO						-13.598	12	.158	14.245	1.0		36.09	
ATO	OM 74					-14.864	11	. 299	14.145	1.0		39.26	
ATC			_			-14.932	10		12.881	1.0		86.61	
ATC		_				-14.762		_	11.601	1.0	_	7.72	
ATO						-15.491	12.	_	11.363	1.0		8.41	
ATO						-13.798			10.770	1.0		7.88	
ATO	M 748	0				13.671			15.451	1.0		7.67	
ATO	M 749		, As			13.150	12.	_	L6.513	1.0		1.28	
ATO	M 751					14.282	14.	_	5.243	1.00		1.37	
ATO	M 752					14.487	15.		6.281	1.00		4.93	
ATON		CG				15.828	15.	_	6.975	1.00		3.05	
ATOM		OD		_		17.007	15.2		6.067	1.00		0.80	
ATOM	1 755	OD:				17.921	16.0		6.491	1.00		.88	
ATOM	756	С	AS			17.016	14.7		4.925	1.00		.89	
ATOM	,	0	ASI			13.367	15.3	66 1	7.316	1.00	- •	. 98	
ATOM	. 30	N	GL		-	L3.556	15.0		3.502	1.00		.04	
MOTA		CA	GLY		_	2.205	15.8		5.860	1.00		.73	
ATOM	761	C	GLY			1.080	15.9		_	1.00		.30	
ATOM	762	0	GLY		_	9.761	15.7	13 17	_	1.00		. 32	
ATOM	763	N	PRO			9.740	15.4	65 15		1.00	40.		
ATOM	764	CD	PRO		-	8.644	15.7	76 17		1.00	40.	71	
ATOM	<b>76</b> 5	CA	PRO		-	8.585	15.98	33 19	22-	1.00	39.		
MOTA	766	CB	PRO	1556	-	7.298	15.56	56 17		1.00	40.		
ATOM	767	CG	PRO	1556		6.405	15.77	1 18		.00	38.		
ATOM	768	C	PRO	1556	- '	7.226	16.57	3 19		.00	38.		
ATOM	769	0	PRO	1556		7.140	14.15	4 16.		.00	41.		
ATOM	770	N	LEU	1557		7.606	13.20	8 17.	_	.00	36.5		
MOTA	772	CA	LEU	1557	-6	.447	14.01	7 15.		:00	37.		
ATOM	773	CB	LEU	1557	- 6	. 201	12.71	9 15.		.00	36.7		
ATOM	774	CG	LEU			. 528	12.88	5 13.	_	.00	34.8		
ATOM	775	CD1	LEU	1557	<del>-</del> 5	.004	11.623	3 12.		. 00	32.4		
ATOM	776	CD2	LEU	1557	-6	.146	10.655	12.		.00	30.8		
ATOM	777	C	LEU	1557	-4	. 283	12.014	11.			26.2		
ATOM	778	ō	LEU	1557		.290	11.925	15.			25.5		
ATOM	779	N	TYR	1557	- 4	.229	12.410	16.			33.6		
ATOM	781	CA	TYR	1558	-5	718	10.724	16.3			33.6		
	•		* 1 K	1558	-4.	902	9.863				31.9	7	
SSSD/551	145. v01								<b>.</b>	00	31.83	L.	





											r
					_ 5	.614	9.500	18.462	1.00	33.	
MOTA	782	CB	TYR	1558		.710	10.638	19.461	1.00	35. 35.	
MOTA	783	CG	TYR	1558		.644	10.608	20.499	1.00		
MOTA	784	CD1	TYR	1558		.757	11.670	21.394	1.00	38.	
MOTA	785	CE1	TYR	1558		. 883	11.759	19.349	1.00	38.	
MOTA	786	CD2	TYR	1558		. 985	12.824	20.235	1.00	40.	
ATOM	787	CE2	TYR	1558		5.924	12.781	21.254	1.00		
ATOM	788	CZ	TYR	1558		5.040	13.867	22.104	1.00		
ATOM	789	OH	TYR	1558		1.607	8.604	16.345	1.00		. 08
MOTA	791	С	TYR	1558		5.527	7.937	15.857	1.00		.28
MOTA	792	0	TYR	1558		3.328	8.336	16.116	1.00		.34
MOTA	793	И	VAL	1559		2.934	7.132	15.403	1.00		.39
MOTA	795	CA	VAL	1559		1.830	7.401	14.364	1.00	_	.17
MOTA	796	CB	VAL	1559		1.463	6.103	13.648	1.00		.25
MOTA	797	CGl	VAL	1559	-	2.297	8.461	13.360	1.00		.56
ATOM	798	CG2	VAL	1559	_	2.411	6.226	16.498	1.0		5.14
MOTA	799	С	VAL	1559	_	1.396	6.522	17.120	1.0	-	3.04
MOTA	800	0	VAL			3.164	5.171	16.783	1.0		5.28
ATOM	801	N	ILE			2.832	4.208	17.831		-	1.81
ATOM	803	CA	ILE			-4.133	3.669	18.496			4.63
ATOM		CB	ILE			-3.790	2.812	19.728			0.93
ATOM	805	CG2				-5.044	4.854	18.869	1.0		2.94
ATOM	806	CG1				-6.499	4.502	19.028	3 1.0		5.34
ATOM		CD1				-1.994	3.051	17.286			6.38 6.14
MOTA		С	ILI			-2.429	2.301	16.39		_	7.31
MOTA	1 809	0	IL			-0.782	2.91	17.80	9 1.0		7.32
MOTA	1 810	N	VA:			0.112	1.852	2 17.35	9 1.		25.01
OTA		CA	VA			1.309	2.43	5 16.52	7 1.	-	19.39
ATO		CB	VA			0.785	3.22	0 15.33			26.08
OTA		CG				2.170	3.34				25.89
ATO		_				0.615	1.02				25.64
ATO			VA			0.364	1.37				24.49
ATO	M 817		VP			1.288	-0.07				25.00
OTA			GI GI			1.806	-0.94			. 00	23.69
ATC				្ស 156		2.357	-2.23	18.6		.00	24.29
ATC				ւՄ 156		1.272	-3.17			.00	27.65
ATC				LU 156		1.814	-4.39			.00	29.50
TA			_	LU 156		1.218	-5.4	80 17.6		.00	32.34
TA		-		LU 150		2.832	-4.2			.00	27.27
TA		_		LU 15		2.840				.00	26.18
TA				LU 15		3.59		_		.00	30.39
TA				YR 15		2.82				.00	32.48
	OM 82				63	3.71				00	33.91
	OM 83				63	2.93				1.00	34.93
	OM 83	-			63	3.78				1.00	34.50
		_			63	4.60				1.00	37.77
			_		63	5.37		)51 25.1	-	1.00	33.54
				-	563	3.75				1.00	34.94
					563	4.51		171 27.		1.00	37.22
		<del>-</del> -			563	5.32	21 1.	296 27.	-	1.00	45.36
		_			563	6.0	37 1.			1.00	31.53
		• •	C		563	4.8	96 -1.		730	1.00	30.43
			0	-	563	4.7			895 761	1.00	32.28
			N		564	6.0	82 -0.	444 22	761		
Ą	MOT.	342	••								

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							-50				
	ATOM	844	CA	ALA	1564	. 7.3					
	ATOM	845	CB		1564			1.167	23.02	5 1.00	32.59
	<b>~</b>	846	C		1564			957	21.863	1.00	
		847	0		1564			608	24.334	1.00	31.81
	<b></b>	848	N		1565	7.61		.427	24.345	1.00	34.11
		B50	CA	~	.565	8.03	_	.296	25.434	1.00	34.09
		351	CB		565	7.40	_	.853	26.763	1.00	35.05
		352	OG		565	7.68		. 725	27.829	1.00	30.13
			C		565	9.52		. 084	27.579	1.00	38.17
			0	~	565	9.32 9.94	_	. 769	27.041	1.00	35.03
			N	• • • •	566	10.32		.001	27.902	1.00	37.12
					566	11.75		557	26.330	1.00	34.55
					566	12.29			26.562	1.00	33.48
					66	11.674			26.508	1.00	31.90
			D 1		66	12.162		865	27.586	1.00	28.63
		•	CE I		66	11.763		287	27.508	1.00	34.97
		<u>-</u> '		YS 15		12.288			28.761	1.00	36.82
AT		_	L	YS 15		12.567	-		28.748	1.00	41.32
AT		_	_	YS 15		13.785			25.691	1.00	34.98
AT			_	LY 15		11.892	-0.1		25.607	1.00	38.03
ATO		_	•	LY 156	57	12.582	0.3		5.049	1.00	36.00
ATO		_	G)	LY 156	57	13.245	1.3		4.222		34.14
ATC		•		ΣY 156	57	12.975	0.8	_	2.933	1.00	32.01
ATO				SN 156	8	14.091	-0.2		2.439		31.95
ATO						14.774	1.7 1.3		2.360		33.51
ATO						15.203	2.6			1.00 3	4.20
ATO						16.420	3.3			1.00 3	4.07
ATO	-	OD ND	_			17.453	2.70			1.00 3	5.09
ATO		C		,		16.317	4.62	_	~	1.00 3	4.36
ATOM	1 884	0	AS		3	15.927	0.40				8.38
ATON		N	ASI	_		16.490	0.31				3.38
ATOM		CA	LE( LE(			16.276	-0.31		262		4.93
ATOM		СВ	LEU			17.333	-1.31		200		l.11
ATOM	889	CG	LEU			17.437	-2.00		^-	.00 30	.44
ATOM	890	CD1				18.438	-3.14			.00 29	46
ATOM		CD2				18.285	-4.21				.01
ATOM	892	С	LEU		1	8.263	-3.74(	17.	_		.81
ATOM	893	0	LEU	1569		8.706	-0.805	20.	~		.62
ATOM	894	N	ARG	1570		9.400	-1.501	21.	455		.16
ATOM	896	CA	ARG	1570		9.097	0.396	20.			. 32
ATOM	897	CB	ARG	1570	2	0.386 0.597	0.951	20.	_ ·	00 33	. 74
ATOM	898	CG	ARG	1570			2.349	20.3		00 32	
ATOM	899	CD	ARG	1570		1.873	3.009	20.6			
ATOM	900	NE	ARG	1570	2.	1.966	4.481	20.3			
ATOM	902	CZ	ARG	1570	20	7.749	5.222	20.6			
ATOM	903	NH1	ARG	1570	21	).376 118	5.600	21.8			
ATOM	906	NH2	ARG	1570	7.0	118	5.316	22.9	60 1.0		
ATOM	909	C	ARG	1570	20	.246	6.284	22.0	33 1.0		
ATOM	910	0	ARG	1570		. 434	1.022	22.2	98 1.0		
ATOM	911	N	GLU	1571		. 324	0.444	22.9	39 1.0		
ATOM	913	CA	GLU	1571		.331	1.695	22.8	80 1.0		
ATOM	914	CB	GLU	1571		. 331	1.835	24.3	28 1.0		
ATOM	915	CG	GLU	1571	18	.055 .061	2.607	24.66	7 1.0		
SSSD/55				-	40.	. 001	4.056	24.20	08 1.0		
~>>U/55	145 VA1								-	,	_

ATOM	916	CD	GLU	1571	16.694	4.721	24.311	1.00	51.36
MOTA	917	OEl	GLU	1571	15.676	3.996	24.417	1.00	55.22
MOTA	918	OE2	GLU	1571	16.635	5.972	24.267	1.00	53.59
MOTA	919	C	GLU	1571	19.314	0.469	25.022	1.00	34.82
ATOM	920	0	GLU	1571	20.018	0.242	26.013	1.00	35.05
MOTA	921	N	TYR	1572	18.520	-0.441	24.469	1.00	33.35
ATOM	923	CA	TYR	1572	18.366	-1.796	24.986	1.00	31.83
MOTA	924	СВ	TYR	1572	17.365	-2.544	24.102	1.00	30.77
ATOM	925	CG	TYR	1572	17.170	-4.008	24.408	1.00	28.50
MOTA	926	CD1	TYR	1572	16.193	-4.420	25.313	1.00	30.48
MOTA	927	CE1	TYR	1572	15.977	-5.760	25.574	1.00	30.97
ATOM	928	CD2	TYR	1572	17.933	-4.985	23.772	1.00	26.14
ATOM	929	CE2	TYR	1572	17.725	-6.329	24.027	1.00	26.21
ATOM	930	CZ	TYR	1572	16.742	-6.708	24.935	1.00	30.30
MOTA	931	OH	TYR	1572	16.518	-8.041	25.214	1.00	33.52
MOTA	933	C	TYR	1572	19.692	-2.556	25.044	1.00	34.83
MOTA	934	0	TYR	1572	19.959	-3.308	25.992	1.00	34.93
MOTA	935	N	LEU	1573	20.517	-2.370	24.020	1.00	34.34
MOTA	937	CA	LEU	1573	21.803	-3.053	23.961	1.00	35.38
MOTA	938	CB	LEU	1573	22.357	-3.027	22.531	1.00	32.71
ATOM	939	CG	LEU	1573	21.669	-3.891	21.464	1.00	29.16
MOTA	940	CD1	LEU	1573	22.161	-3.503	20.087	1.00	26.98
ATOM	941	CD2	LEU	1573	21.932	-5.351	21.710	1.00	28.85
MOTA	942	С	LEU	1573	22. <b>79</b> 9	-2.420	24.933	1.00	37.54
MOTA	943	0	LEU	1573	23.511	-3.123	25.659	1.00	36.67
MOTA	944	N	GLN	1574	22.814	-1.092	24.969	1.00	37.90
MOTA	946	CA	GLN	1574	23.729	-0.368	25.838	1.00	39.77
ATOM	947	CB	GLN	1574	23.624	1.138	25.572	1.00	40.09
ATOM	948	CG	GLN	1574	24.208	1.549	24.217	1.00	42.28
ATOM	949	CD	GLN	1574	24.030	3.018	23.896	1.00	44.28
MOTA	<del>9</del> 50	OE1	GLN	1574	23.362	3.755	24.615	1.00	47.55
ATOM	951	NE2	GLN	1574	24.613	3.448	22. <b>79</b> 0	1.00	46.09
ATOM	954	С	GLN	1574	23.490	-0.697	27.310	1.00	40.75
MOTA	955	0	GLN	1574	24.440	-0.939	28.059	1.00	41.29
ATOM	956	N	ALA	1575	22.220	-0.783	27.696	1.00	40.10
ATOM	958	CA	ALA	1575	21.842	-1.088	29.069	1.00	38.81
ATOM	959	CB	ALA	1575	20.349	-0.819	29.273	1.00	35.69
ATOM	960	C	ALA	1575	22.192	-2.514	29.503	1.00	40.63
ATOM	961	0	ALA	1575	22.098	-2.843	30.690	1.00	43.39
ATOM ATOM	962	N	ARG	1576	22.602	-3.357	28.561	1.00	38.39
	964	CA	ARG	1576	22.945	-4.729	28.896	1.00	37.69
MOTA MOTA	965 966	CB	ARG	1576	22.034	-5.689	28.137	1.00	38.16
	966	CG	ARG	1576	20.594	-5.547	28.589	1.00	37.89
ATOM ATOM	967	CD	ARG	1576	19.622	-6.281	27.711	1.00	37.36
ATOM	968 970	NE CZ	ARG	1576	18.267	-6.255	28.265	1.00	34.99
ATOM	971	CZ	ARG	1576	17.565	-5.150	28.484	1.00	36.94
		NH1	ARG	1576	18.083	-3.960	28.209	1.00	36.18
ATOM	974	NH2	ARG	1576	16.310	-5.237	28.909	1.00	40.93
ATOM	977	C	ARG	1576	24.413	-5.073	28.704	1.00	38.93
ATOM ATOM	978	O	ARG	1576	24.801	-6.249	28.699	1.00	39.75
	979	N CD	ARG	1577	25.233	-4.036	28.570	1.00	39.21
ATOM	981	CA	ARG	1577	26.671	-4.196	28.413	1.00	38.97
ATOM	982	CB	ARG	1577	27.307	-2.870	28.000	1.00	36.06
ATOM	983	CG	ARG	1577	26.992	-2.408	26.610	1.00	36.41



			CD AI	RG 1577	27.69	95 -1.09	24 05 5-	_	
	OM 98	_	VE AI	RG 1577					
AT		_	ZZ AF					00	38.45
AT		18 <i>V</i>	THI AF						39.00
AT		1 N	TH2 AR						38.88
AT(		4 C			27.24				37.76
ATO		_	AR		26.68				40.59
ATO		6 <b>N</b>	PR		28.35				38.52
ATC		7 C.	D PR		29.07	· ·			43.19
ATC		B C	A PR		28.95	·			44.84
ATO		9 <b>C</b> 1	B PR		30.06				45.06
ATO		00 C	3 PR		30.43				44.86
ATO		oi c	PRO		29.51				44.56
ATO		02 0	PRO		29.809				44.93
ATO		)3 N	PRO		29.649				43.13
ATO	M 100	4 CI			29.315				47.61
ATO		5 CA			30.173				48.39
ATO		6 CB			30.173				48.74
ATO		7 CG			29.027				49.73
MOTA	4 100	8 C	PRO		31.591			1.00	49.21
ATOM	1 100	9 0	PRO		32.483			1.00	49.67
ATOM		0 N	GLU		19.165		33.361	1.00	52.07
ATOM		2 CA			20.603		32.444	1.00	64.83
ATOM		3 CB	GLU		20.803	-5.147	32.491	1.00	64.82
ATOM	1014	4 C	GLU	1592	20.969	-4.421	33.784	1.00	67.61
ATOM		5 0	GLU	1592	22.653	-6.413	32.335	1.00	63.99
ATOM		N	GLU	1593	20.821	-6.336	32.098	1.00	65.67
MOTA			GLU	1593	21.534	-7.575	32.485	1.00	62.41
ATOM	~~	CB	GLU	1593	20.595	-8.844	32.342		61.23
ATOM	1020	C	GLU	1593	22.141	-10.017	32.600		61.20
ATOM	1021	0	GLU	1593	21.494	-8.953	30.944	1.00	59.26
ATOM	1022	N	GLN	1594	23.388	-8.631	29.945	1.00	59.84
ATOM	1024	CA	GLN	1594	24.101	-9.405	30.888	1.00	57.94
ATOM	1025	CB	GLN	1594	25.501	-9.558	29.625	1.00	54.91
ATOM	1026	CG	GLN	1594	26.439	-10.141	29.865		55.13
ATOM	1027	CD	GLN	1594	27.682	-9.252	30.679	1.00	56.93
ATOM	1028	OE1	GLN	1594	28.241	-9.997	31.180	1.00	9.60
ATOM	1029	NE2	GLN	1594	28.117	-10.858	30.488	1.00 5	8.45
ATOM	1032	C	GLN	1594	23.331	-9.662	32.393	1.00 5	8.95
ATOM	1033	0	GLN	1594	22.637	-10.438	28.640		2.30
ATOM	1034	N	LEU	1595	23.438	-11.389	29.025	1.00 5	2.03
ATOM	1036	CA	LEU	1595	22.782	-10.091	27.366		9.60
ATOM	1037	CB	LEU	1595	22.459	-10.836	26.308	1.00 4	5.16
ATOM	1038	CG	LEU	1595	21.463	-9.907	25.135	1.00 4	1.36
ATOM	1039	CD1	LEU	1595	21.617	-8.815	25.523		9.43
MOTA	1040	CD2	LEU	1595	20.060	-7.583	24.644		6.21
ATOM	1041	C	LEU		23.747		25.480	1.00 3	4.91
ATOM	1042	0			24.953				3.30
ATOM	1043	N	SER		23.230			1.00 43	3.62
MOTA	1045	CA			23.230 24.085		25.553		2.92
ATOM	1046	СВ							. 86
ATOM	1047	OG							.86
MOTA	1049	C							.88
MOTA	1050	0						_	. 59
					23.657	-13.077	22.966		. 94

ATOM	1051	N	SER	1597	25.275	-14.637	23.018	1.00	39.60	
ATOM	1053	CA	SER	1597	25.557	-14.518	21.603	1.00	39.74	
ATOM	1054	CB	SER	1597	26.729	-15.409	21.223	1.00	41.38	
ATOM	1055	OG	SER	1597	27.824	-15.147	22.077	1.00	50.59	
ATOM	1057	С	SER	1597	24.315	-14.921	20.818	1.00	38.16	
MOTA	1058	0	SER	1597	24.036	-14.353	19.769	1.00	38.03	
ATOM	1059	N	LYS	1598	23.560	-15.891	21.327	1.00	36.40	
ATOM	1061	CA	LYS	1598	22.362	-16.312	20.634	1.00	35.97	
ATOM	1062	СВ	LYS	1598	21.791	-17.594	21.228	1.00	36.69	
MOTA	1063	CG	LYS	1598	20.989	-18.402	20.198	1.00	40.42	
MOTA	1064	CD	LYS	1598	20.164	-19.499	20.838	1.00	40.37	
MOTA	1065	CE	LYS	1598	19.792	-20.572	19.829	1.00	46.34	
ATOM	1066	NZ	LYS	1598	20.993	-21.338	19.362	1.00	45.29	
ATOM	1070	С	LYS	1598	21.324	-15.194	20.696	1.00	37.49	
ATOM	1071	0	LYS	1598	20.567	-14.983	19.738	1.00	38.10	
ATOM	1072	N	ASP	1599	21.316	-14.458	21.807	1.00	35.21	
MOTA	1074	CA	ASP	1599	20.380	-13.352	21.983	1.00	34.02	
MOTA	1075	CB	ASP	1599	20.556	-12.686	23.346	1.00	37.78	
ATOM	1076	CG	ASP	1599	19.970	-13.493	24.483	1.00	40.05	
MOTA	1077	OD1	ASP	1599	20.270	-13.143	25.642	1.00	42.73	
ATOM	1078	OD2	ASP	1599	19.204	-14.450	24.235	1.00	42.39	
ATOM	1079	С	ASP	1599	20.633	-12.306	20.922	1.00	32.84	
MOTA	1080	0	ASP	1599	19.694	-11.779	20.311	1.00	30.59	
ATOM	1081	N	LEU	1600	21.912	-11.999	20.724	1.00	31.11	
ATOM	1083	CA	LEU	1600	22.323	-10.998	19.744	1.00	32.17	
ATOM	1084	CB	LEU	1600	23.823	-10.722	19.875	1.00	32.30	
MOTA	1085	CG	LEU	1600	24.275	-10.162	21.235	1.00	31.08	
ATOM	1086	CD1	LEU	1600	25.794	-9.931	21.242	1.00	30.59	
ATOM	1087	CD2	LEU	1600	23.549	-8.863	21.514	1.00	28.89	
ATOM	1088	С	LEU	1600	21.949	-11.390	18.311	1.00	30.77	
MOTA	1089	0	LEU	1600	21.352	-10.601	17.574	1.00	29.87	
ATOM	1090	N	VAL	1601	22.269	-12.623	17.933	1.00	30.19	
ATOM	1092	CA	VAL	1601	21.954	-13.115	16.602	1.00	29.25	
MOTA	1093	CB	VAL	1601	22.593	-14.497	16.349	1.00	31.27	
MOTA	1094	CG1	VAL	1601	22.355	-14.936	14.914	1.00	31.60	
MOTA	1095	CG2	VAL	1601	24.093	-14.434	16.622	1.00	31.91	
ATOM	1096	С	VAL	1601	20.438	-13.181	16.405	1.00	29.06	
MOTA	1097	0	VAL	1601	19.946	-12.914	15.310	1.00	27.71	
ATOM	1098	N	SER	1602	19.702	-13.511	17.468	1.00	29.10	
MOTA	1100	CA	SER	1602	18.243	-13.585	17.400	1.00	29.29	
ATOM	1101	CB	SER	1602	17.680	-14.189	18.679	1.00	30.81	
ATOM	1102	OG	SER	1602	16.266	-14.074	18.692	1.00	35.78	
ATOM	1104	C	SER	1602	17.649	-12.199	17.156	1.00	28.98	
MOTA	1105	0	SER	1602	16. <b>66</b> 2	-12.039	16.426	1.00	26.82	
MOTA	1106	N	CYS	1603	18.274	-11.202	17.765	1.00	29.06	
ATOM	1108	CA	CYS	1603	17.870	-9.823	17.599	1.00	29.22	
ATOM	1109	CB	CYS	1603	18.784	-8.943	18.438	1.00	29.66	
ATOM	1110	SG	CYS	1603	18.575	-7.212	18.103	0.50	23.69	PRT1
ATOM	1111	С	CYS	1603	17.988	-9.422	16.112	1.00	29.23	
MOTA	1112	0	CYS	1603	17.087	-8.796	15.552	1.00	27.52	
MOTA	1113	N	ALA	1604	19.113	-9.778	15.491	1.00	27.87	
MOTA	1115	CA	ALA	1604	19.376	-9.484	14.077	1.00	26.37	
MOTA	1116	CB	ALA	1604	20.783	-9.941	13.690	1.00	23.88	
MOTA	1117	С	ALA	1604	18.349	-10.203	13.223	1.00	25.82	

							134				
	ATOM	1118	0	ALA	1604						
	ATOM	1119	N	TYR		<i></i>		9.631	12.289	1.00	25.0.
	ATOM	1121	CA	TYR	1605			1.468	13.544		-0.04
	ATOM	1122	CB	TYR	1605		l52 -12	2.276	12.827		
	ATOM	1123	CG	TYR	1605		080, - <u>1</u> 3	3.662	13.456		27.81
7	ATOM	1124	CD1	TYR	1605	15.9	74 -14	.515	12.886	-	26.66
7	ATOM	1125	CE1		1605	16.1	11 -15	.141	11.640		30.75
1		1126	CD2	TYR	1605	15.0	88 -15	. 944	11.126	1.00	30.20
P	moss	1127	CE2	TYR	1605	14.7	90 -14	.707		1.00	30.03
A		1128	CZ		1605	13.7	75 -15	.500	13.596	1.00	30.73
A					1605	13.93		.117	13.097	1.00	30.71
	ma		OH		1605	12.92			11.867	1.00	30.93
	_	1 2 2	^		1605	15.74			11.417	1.00	32.31
				TYR :	1605	15.14			12.775	1.00	26.15
				GLN ;	1606	15.24			11.702	1.00	26.64
			CA (		1606	13.92			13.926	1.00	25.48
	no.		CB (		606			581	14.023	1.00	26.86
					606	13.58	-	269 j	15.482	1.00	
		138 (	~~		606	13.35		508 ]	6.332		26.83
		139 c				13.15	1 -11.		7.791		25.84
	'OM 11		_	_	606	12.202	2 -10.4		8.150	1.00	30.86
AT	OM 11	43 C			606	14.056	-11.6		8.640	1.00	31.87
AT	OM 11	44 0	•		606	13.835	-9.3		3.186		31.67
AT	<b>~</b> • •	45 N	_		606	12.831	-9.C		^ =		27.52
ATO	OM 11		_		507	14.904				1.00	26.05
ATO		4.0			507	14.963			_	1.00 2	26.68
ATO					07	16.225	-6.4		2.435		5.66
ATC	-	_			07	16.363			2.787		8.50
ATO			32 V	L 16	07	16.151			853		6.04
ATO			VA	L 16	07	14.934	-6.0		.246		4.45
ATO		_	VA			14.184	-7.64				4.89
			AL			15.738	-7.03				5.86
ATO		-	AL				-8.61				5.24
ATO		6 CB	AL			15.773	-9.03	و وا			
ATO	_	7 C	AL			16.813	-10.11	.7 g			2.95
ATO		8 0	AL			14.383	-9.54	1 8.	~		.24
ATOM		9 N	ARC			13.963	-9.31	9 7.			. 71
ATOM			ARG		-	13.676	-10.21	_			.48
ATOM		CB	ARG		_	L2.327	-10.70		_		.10
ATOM	1163		ARG		_	1.840	-11.64				.55
ATOM	1164					.2.407	-13.009		_		. 53
ATOM	1165		ARG			1.537	-13.93]	11.		00 36	.05
ATOM			ARG			0.849	-14.874				. 28
ATOM	,		ARG	1609		9.974	-15.771			00 42	. 06
ATOM	1171		ARG	1609	•	9.678	-15.834		532 1.	00 42.	08
ATOM	1174		ARG	1609		_	-16 620	-	928 1.	00 40.	
ATOM		С	ARG	1609	1:	1.329	-16.620			00 43.	
ATOM	1175	0	ARG	1609	10	0.469	-9.569			00 25.	
	1176	N	GLY	1610		418	-9.621	8.2	31 1.0		
ATOM	1178	CA	GLY	1610		 	-8.565	9.9	96 1.(		
ATOM	1179	C	GLY	1610		.555	-7.406	9.8			
ATOM	1180	0	GLY	1610		.800	-6.747	8.5	_		
ATOM	1181	N	MET			.855	-6.424	7.7			<b>7</b> ∠
ATOM	1183	CA	MET	1611	12	.076	-6.589	8.1		• •	
ATOM	1184	CB		1611	12	.456	-5.989	6.8		-5.1	
ATOM	1185	CG	MET	1611	13	. 956	-5.710	6.84			
ATOM	1186		MET	1611	14	.398	-4.542				
		SD	MET	1611	13.		-3.006	7.72	_	0	
SSSD/55	145						500	7.42	1.0	25.2	3
. =, 33	, 43. VU [										



										- 00	21.38	3
					13.	912	-2.6	88	5.675	1.00	23.90	, 5
T COM	1187	CE	MET	1611	12.	050	-6.8		5.681	1.00	25.2	5
MOTA	1188	С	MET	1611	11.	673	-6.3		4.633	1.00	_	4
MOTA	1189	0	MET	1611			-8.1		5.822	1.00	_	- -
MOTA	1190	N	GLU	1612	12.	130	-9.0		4.733	1.00		
ATOM		CA	GLU	1612	11.	755	-10.4	194	5.121	1.00		
MOTA	1192	CB	GLU	1612	12.	018	-11.4	1 D Q	4.009	1.00	26.7	
MOTA	1193		GLU	1612	11.	703			4.450	1.00	26.9	
MOTA	1194	CG	GLU	1612	11	.812	-12.	931	5.636	1.00	30.9	98
MOTA	1195	CD		1612	11	.557	-13.	212	3.61		ე 32.∷	31
MOTA	1196	OE1	GLU	1612	12	.154	-13.		4.41			70
MOTA	1197	OE2	GLU	1612	10	.267		829				30
MOTA	1198	С	GLU			.860		753	3.25	_		55
MOTA	1199	0	GLU	1612		.463	-8.	723	5.46			
MOTA	1200	N	TYR	1613		.037	-8	501	5.29	-		00
ATOM		CA	TYR	1613	-	7.314	- 8	.586	6.65			93
			TYR	1613		5.841		.281	6.54	9 1.0		60
MOTA			TYR	1613			- 9	.245	6.09			14
MOTA			TYR	1613		4.945	- 8	.962	5.96	3 1.0	-	. 14
ATOM				1613		3.582	7	.018	6.86	59 1.		. 81
MOTA						5.347		.718	6.73	33 1.	-	.45
MOTA						3.979		1.697	6.2		00 23	.28
OTA			TYI			3.112			6.1	26 1.	00 22	.95
OTA					,	1.775		7.411	4.6		00 22	.57
ATO			TY			7.803		7.138	3.6		00 24	.72
ATO	M 121					7.022		7.024		_	.00 22	2.16
OTA	M 121		TY			8.460		6.101	_		.00 23	2.60
ATO			LE			8.334	-	4.755			.00 2	2.56
ATC	M 123			-		9.175	5 -	3.772		_	.00 2	4.92
ATC						8.57	7 -	3.415		,	.00 2	1.46
ATO		18 CC				9.53	5 -	2.541			.00 2	1.87
TA	_	19 CI		EU 161		7.21	8 -	2.711			00 2	3.76
ATC			_	EU 161		8.69	9 .	4.683	-		00 2	3.84
AT		21 C		EU 161		7.97		-4.07				3.48
		22 0		EU 163		9.80		-5.31	42.			22.70
	-	223 N	A	LA 16		10.23	-	-5.34	01.			21.52
			A A	LA 16		11.59		-6.01	9 1.	. — -		22.87
		226	B P	LA 16		9.18	90	-6.06	3 0		_	24.23
				LA 16				-5.59	-0	. • •		22.76
			0 1	LA 16	15	8.8		-7.17	76 1	• -		22.76
	_	220			16	8.6		-7.95	54 0	. 295	1.00	
					16	7.6		-9.2	51 1	.039	1.00	21.39
				SER 16	516	7.3		-9.0	_	.102	1.00	26.24
			_		616	6.4	.00	-7.1		.044	1.00	24.88
			C		616	6.3	160	-7.3		.927	1.00	24.73
		1235	0		616	5.6	335	-1.3		927	1.00	23.82
1		1236			617	6.1		-6.1		0.810	1.00	22.47
1		1237	N	_	617		970	-5.2		2.199	1.00	23.62
i		1239	CA		617		455	-4.9		2.927	1.00	27.16
•	MOTA	1240	CB	_	617		792	-6.0		2.169	1.00	30.84
	MOTA	1241	CG		1617		551	' -6.4		2.109	1.00	33.57
	MOTA	1242	CD		1617	1.	810	-7.	•	2.852	1.00	44.30
-	MOTA	1243	CE			2.	484	-8.		2.653	1.00	23.56
-	MOTA	1244	NZ		1617		346	-4.	034	0.035		25.16
	MOTA	1248	С	_	1617		.639	-3.	030	0.091	1.00	24.69
	MOTA	1249	0		1617		.495		066	-0.638	1.00	
		1250	N	LYS	1618		.953		943	-1.468	1.00	24.04
	ATOM	1252	CA	LYS	1618	6	. 533					
	MOTA											

							136				
	ATOM		3 CB	IVC							
	ATOM		4 CG	LYS	1618	5.8	63 _	2.581			
	ATOM	125		LYS	1618	5.7		2.581	-2.492	1.00	26.96
	ATOM	1256		LYS	1618	5.5	_	3.491	-3.709	1.00	
	ATOM	1257		LYS	1618	5.66	_	4.942	-3.345	1.00	29.14
	ATOM			LYS	1618			5.858	-4.558		33.91
	ATOM	1261	_	LYS	1618	4.43		5.821	-5.380	1.00	32.98
		1262	0	LYS	1618	7.40	6 -1		-0.713	1.00	36.73
	ATOM	1263	N	CYS		7.55	7 -0			1.00	24.01
	ATOM	1265	CA		1619	7.68	9 -1	.842	-1.302	1.00	23.73
	ATOM	1266	CB	CYS	1619	8.10	. –	77.	0.573	1.00	25.91
	ATOM	1267		CYS	1619	7.444		.731	1.418	_	25.51
	ATOM	1268	SG	CYS	1619	7.941		.885	2.792	_	25.65
	ATOM		C	CYS	1619		-	. 313	4.064	_	24.93
	ATOM	1269	0		1619	9.631	-0.		_	1.00	28.14
	_	1270	N	**		10.304	- 1		1	1.00	23.07
	ATOM	1272	CA		1620	10.170	` O.	~		1.00 2	0.98
	MOT	1273	CB		1620	11.604			1.363	1.00 2	2.95
	MOT	1274	CG2		1620	12.202			.524	1.00 2	3.81
A		1275			1620	13.670		607 o	.276	1.00 2	7.01
	mo.	1276	CG1	ILE 1	.620	12.108		995 <sub>0</sub>		_	4.36
	mo		CD1	T	620	12.108	0.5	739 <sub>-0</sub>			7.24
	770.0	1277	C	<b>*</b>	620	12.171	1.5	44 -2		.00 2	3.13
		278	^		_	11.633	1.7				5.37
		279				10.981	2.7			.00 24	.70
AT		281 (	~~		521	12.348	1.2			.00 25	.21
AT	OM 1	200	~~ ·		521	12.427	2.0		804 1	.00 25	.62
AT	'OM 1:	202	· ·		21	13.181	1 2	_	057 1		.53
ΤA		_	-	IS 16	21 :	13.004	1.2	6.		_	. 76
AT	~··	·		IS 16	21 ]	12.356	1.77				. 76
ATO				IS 16	21 1	3 434	1.26	io 8.			42
ATO			E1 H.	IS 16:	_	3.474	3.01		`	- •	
ATO	<b></b>	88 N	E2 H	IS 16:	. ~	3.119	3.23				62
	<del>-</del>		H)		_	2.439	2.18				70
ATO		91 0	н			3.073	3.40			<sup>00</sup> 26.	23
ATO		92 N				2.528	4.40	_		00 26.	
ATO			AR	~	2 14	1.271			70 1.0	0 25.8	
ATO	M 129			-02	2 19	5.082	3.406		41 1.0		9
ATO					2. 14	.268	4.608	4.1	40 1.0		
ATOM		_		G 162:	2 12	.709	5.766	3.54			5
ATOM			AR			. 709	5.444	2.17			9
ATOM		-1-2	ARC			.089	6.656	1.48			
	- •	- 2	ARG			.684	6.300	0.13		~ 1.0	6
ATOM						.606	5.577	-0.13	-		5
ATOM	1304	4 NH2		2		801	5.137	-0.16		11.8	3
ATOM	1307				11.	366	5.239	0.79		10.20	
ATOM	1308		ARG		15.	877		-1.42		8.63	
ATOM	1309	_	ARG		16.		5.058	5.379	9 1.00		'
ATOM	1311		ASP	1623	15.		5.863	5.268	3 1.00	,	
ATOM			ASP	1623	16	<b>~</b>	4.527	6.552	1.00		
ATOM	1312	CB	ASP	1623	16.		4.899	7.748		24.61	
ATOM	1313	CG	ASP	1623	15.	777 (	5.173	8.410		28.82	
	1314	OD1	ASP		16.	/33 6	735			32.33	
ATOM	1315	OD2	ASP	1623	16.2	276 <del>-</del>	.520	9.469		36.67	
ATOM	1316	C		1623	17.9	37 6	.385	10.321	1.00	43.56	
ATOM	1317	ō	ASP	1623	16.4		766	9.463	1.00	36.29	
ATOM	1318		ASP	1623	16.1		.766	8.766	1.00	28.22	
ATOM		N	LEU	1624	16.7	_	. 937	9.956	1.00	20.42	
ATOM	1320	CA	LEU	1624	16 0	_	. 592	8.278	1.00	26.87	
ATOM	1321	CB	LEU	1624	16.9	_	. 428	9.132		26.34	
T OM	1322	CG	LEU	1624	16.99	96 0	168	8.265	1.00	26.59	
CCC-				~024	17.08	32 -1.	175		1.00	24.59	
SSSD/5.51	45. v01						•	8.978	1.00	24.72	*
										-	

MOTA 1323 CD1 LEU 1624 15.844 -1.408 9.856 1.00 24.35 ATOM 1324 CD2 LEU 1624 17.258 -2.261 7.931 1.00 24.63 MOTA 1325 C LEU 1624 18.210 1.595 10.004 1.00 26.87 MOTA 1326 LEU 0 1624 19.322 1.777 9.497 1.00 28.19 ATOM 1327 N ALA 1625 18.009 1.570 11.317 1.00 27.77 MOTA 1329 CA ALA 1625 19.069 1.741 12.309 1.00 24.54 **ATOM** 1330 CB ALA 1625 19.355 3.210 12.494 1.00 19.81 MOTA 1331 С ALA 1625 18.498 1.173 13.592 1.00 26.44 MOTA 1332 0 ALA 1625 17.289 13.679 0.961 1.00 27.58 MOTA 1333 N ALA 1626 19.342 0.940 14.594 1.00 25.38 MOTA 1335 CA ALA 1626 18.872 0.397 15.865 1.00 24.65 MOTA 1336 CB ALA 1626 20.054 0.023 16.774 1.00 23.35 ATOM 1337 С ALA 1626 17.929 1.373 16.578 1.00 25.54 MOTA 1338 0 ALA 1626 17.057 0.951 17.325 1.00 27.70 ATOM 1339 N ARG 1627 18.104 2.671 16.344 1.00 25.06 ATOM 1341 CA ARG 1627 17.242 3.675 16.959 1.00 25.48 MOTA 1342 CB ARG 1627 17.706 5.089 16.597 1.00 28.15 MOTA 1343 CG ARG 1627 17.759 5.370 15.084 1.00 33.13 ATOM 1344 CD ARG 1627 6.811 18.157 14.774 1.00 33.29 MOTA 1345 NE ARG 1627 18.442 7.011 13.351 1.00 35.74 CZMOTA 1347 ARG 1627 19.652 6.889 1.00 . 37.40 12.813 MOTA 1348 NH1 ARG 1627 20.695 6.585 13.575 1.00 39.73 **ATOM** 1351 NH2 ARG 1627 19.817 7.012 11.507 1.00 36.90 MOTA 1354 С ARG 1627 15.812 3.491 16.479 1.00 24.81 MOTA 1355 0 ARG 1627 14.871 3.853 17.173 1.00 24.05 MOTA 1356 N ASN 1628 15.667 2.910 15.293 1.00 24.80 MOTA 1358 ÇA ASN 1628 14.368 2.686 14.685 1.00 25.97 ATOM 1359 CB ASN 1628 14.383 3.132 13.225 1.00 30.08 MOTA 1360 CG ASN 1628 14.417 4.640 13.096 1.00 33.62 MOTA 1361 OD1 ASN 1628 13.775 5.347 13.864 1.00 35.11 MOTA 1362 ND2 ASN 1.00 1628 15.212 5.141 12.169 36.31 MOTA 1365 С ASN 1628 13.802 1.288 14.824 1.00 26.03 MOTA 1366 0 ASN 1628 12.951 0.869 14.031 1.00 26.87 MOTA 1367 N VAL 1629 14.330 0.550 15.797 1.00 26.04 MOTA 1369 CA VAL 1629 13.854 -0.783 16.128 1.00 25.09 MOTA 1370 CB VAL 1629 14.924 -1.876 15.959 1.00 27.00 MOTA 1371 CG1 VAL 1629 -3.197 14.390 16.546 1.00 20.99 MOTA 1372 CG2 VAL 1629 15.295 -2.051 14.462 1.00 23.26 MOTA 1373 C VAL 1629 13.504 -0.671 17.600 1.00 27.59 ATOM 1374 0 VAL 1629 14.340 -0.285 18.418 1.00 25.81 MOTA 1375 N LEU 1630 12.245 -0.929 17.923 1.00 28.17 ATOM 1377 CA LEU 1630 11.768 -0.845 19.296 1.00 30.20 **ATOM** 1378 CB LEU 1630 10.445 -0.077 19.332 1.00 30.26 ATOM 1379 CG LEU 1630 10.484 1.285 18.626 1.00 29.81 MOTA 1380 CD1 LEU 1630 9.119 1.983 18.745 1.00 28.46 MOTA 1381 CD2 LEU 1630 11.576 2.141 19.233 1.00 28.37 MOTA 1382 C LEU 1630 11.639 -2.242 19.904 1.00 29.32 MOTA 1383 0 LEU 1630 11.414 -3.219 19.189 1.00 30.84 MOTA 1384 N VAL 1631 11.800 -2.342 21.221 1.00 28.90 **ATOM** 1386 CA -3.629 VAL 1631 11.732 21.905 1.00 26.84 MOTA 1387 CB VAL 1631 13.067 -3.919 22.670 1.00 28.88 ATOM 1388 CG1 VAL 1631 13.077 -5.341 23.236 1.00 21.54 MOTA 1389 CG2 VAL 1631 14.259 -3.699 21.744 1.00 24.30 MOTA 1390 C VAL 1631 10.561 -3.645 22.881 1.00 29.02

1	ATOM :	1391	0	178 -								
Į		1392	И	VAL	163			-2.	737 23	3.706	1 00	
A		394	CA	THR	1632		33	-4.6		.764	1.00	
A		395		THR	1632		62	-4.8		.616	1.00	30.84
A		396		THR	1632	-		-5.6		.912	1.00	32.24
		398		THR	1632			-7.0		.910	1.00	31.45
			_	THR	1632		58	-5.1		.470	1.00	30.86
			_	THR	1632	8.91	19	-5.4		.943	1.00	28.04
				THR	1632	10.01		-6.0		. 105	1.00	34.17
				SLU	1633	7.95		-5.5			1.00	35.02
				LU	1633	8.15	5	-6.1		866	1.00	36.16
				LU	1633	6.86		-6.06		177	1.00	36.34
					1633	6.95		-6.64		996	1.00	37.07
					1633	8.03		-6.00		414	1.00	44.57
AT					1633	8.12		-4.75		301	1.00	49.38
AT					1633	8.78		-6.75			1.00	51.03
AT					1633	8.600		-7.58			1.00	51.63
ATO					1633	9.347		-8.08	-		1.00	36.42
ATO			-		1634	8.185		-8.24			1.00	38.56
ATO				_	L634	8.550		-9.63			1.00	37.70
ATO				_	634	7.408		-10.37		737	1.00	38.53
ATO		_		P 1	634	6.041		-10.106			1.00	44.08
ATO		_	D1 AS		634	5.865		-10.36	-		1.00	51.60
ATO				_	634	5.137		-9.631			1.00	52.37
ATO			AS	_	634	9.826		-9.776			1.00	57.23
ATO	<b>-</b>	_	AS	_	634	10.127		10.865			1.00	36.56
ATO		_	AS	_	635	10.569		-8.683			1.00	36.74
ATO		_			535	11.819		-8.662			00	36.56
ATO					535	12.888		-9.587				37.10
ATON					35	13.226		-9.226				16.92
ATON					35	13.275		-8.058	25.91			6.54
ATOM					35	13.423	_	10.235	26.34			8.84
ATOM		_	ASN		35	11.632		-8.980	26.80			9.58
ATOM		_	ASN		35	12.446		-9.677	22.45			4.78
ATOM			VAL		36	10.533		8.498	21.83			4.00
ATOM			VAL			10.279		8.711	21.88			1.35
ATOM		CB	VAL			8.778		8.946	20.46			9.76
ATOM		CG1	****	16:		8.538		9.081	20.18	_		0.60
ATOM	1436 1437	CG2		16:		8.315		0.209	18.67			0.38
ATOM	1438	C	VAL	163	36	10.768		7.449	20.89		00 2	3.51
ATOM	1439	0	VAL	163	36	10.506		6.351	19.78; 20.254			1.02
ATOM	1441	N	MET	163	17	11.575		7.624				.87
ATOM		CA	MET	163	7	12.119	_	6.508	18.738			.15
ATOM	1442	CB	MET	163	7	13.366		6.953	17.980		_	.01
ATOM	1443	CG	MET	163		14.479		7.554	17.204			.82
ATOM	1444	SD	MET	163		L5.124		5.410	18.051			.73
ATOM	1445	CE	MET	163		15.120		7.459	19.288			. 96
ATOM	1446	С	MET	163	7 ]	1.040		. <del>4</del> 39 5.087	20.689			.19
	1447	0	MET	163	7 1	0.480			16.993	1.0	0 24	. 77
ATOM ATOM	1448	N	LYS	1638	_	0.755		791	16.303	1.0	0 24	
	1450	CA	LYS	1638		9.746		.791	16.931	1.0	0 25	
ATOM	1451	CB	LYS	1638		8.486		.258	16.029	1.0		
ATOM	1452	CG	LYS	1638		7.715			16.799	1.0		
ATOM	1453	CD	LYS	1638		6.406			17.298	1.0		
ATOM	1454	CE	LYS	1638		5.486			18.005	1.0	0 23.	
\$\$\$D/55					•		- 5	. 897	18.256	1.0	0 23.	

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ATOM	1455	NZ	LYS	1638	4.871	-6.398	16.976	1.00	24.60
ATOM	1459	С	LYS	1638	10.260	-3.042	15.293	1.00	24.37
ATOM	1460	0	LYS	1638	10.658	-2.055	15.901	1.00	26.58
MOTA	1461	N	ILE	1639	10.271	-3.119	13.971	1.00	25.69
ATOM	1463	CA	ILE	1639	10.721	-2.005	13.148	1.00	25.94
ATOM	1464	CB	ILE	1639	10.935	-2.447	11.668	1.00	26.49
ATOM	1465	CG2	ILE	1639	11.218	-1.236	10.762	1.00	21.19
ATOM	1466	CG1	ILE	1639	12.103	-3.433	11.604	1.00	27.58
MOTA	1467	CD1	ILE	1639	12.120	-4.232	10.355	1.00	32.96
ATOM	1468	C	ILE	1639	9.675	-0.892	13.242	1.00	27.32
MOTA	1469	0	ILE	1639	8.466	-1.133	13.103	1.00	25.45
MOTA	1470	N	ALA	1640	10.156	0.320	13.498	1.00	27.43
ATOM	1472	CA	ALA	1640	9.321	1.499	13.632	1.00	26.96
MOTA	1473	CB	ALA	1640	9.557	2.133	15.006	1.00	25.21
MOTA	1474	С	ALA	1640	9.641	2.510	12.538	1.00	26.80
ATOM	1475	0	ALA	1640	10.691	2.446	11.896	1.00	27.55
ATOM	1476	N	ASP	1641	8.716	3.440	12.328	1.00	27.06
ATOM	1478	CA	ASP	1641	8.862	4.526	11.349	1.00	30.54
MOTA	1479	CB	ASP	1641	9.993	5.484	11.753	1.00	33.12
MOTA	1480	CG	ASP	1641	9.668	6.310	12.999	1.00	36.17
ATOM	1481	OD1	ASP	1641	10.477	7.203	13.334	1.00	42.24
ATOM	1482	OD2	ASP	1641	8.633	6.076	13.648	1.00	33.22
ATOM	1483	С	ASP	1641	9.049	4.107	9.898	1.00	29.94
ATOM	1484	0	ASP	1641	9.598	4.861	9.102	1.00	30.13
ATOM	1485	N	PHE	1642	8.569	2.920	9.553	1.00	30.22
ATOM	1487	CA	PHE	1642	8.680	2.426	8.191	1.00	30.91
ATOM	1488	CB	PHE	1642	8.462	0.909	8.159	1.00	26.24
ATOM	1489	CG	PHE	1642	7.156	0.470	8.750	1.00	27.82
ATOM	1490	CD1	PHE	1642	5.986	0.495	7.988	1.00	27.08
ATOM	1491	CD2	PHE	1642	7.089	0.026	10.066	1.00	26.70
ATOM	1492	CE1	PHE	1642	4.761	0.088	8.532	1.00	25.18
ATOM	1493	CE2	PHE	1642	5.872	-0.383	10.624	1.00	27.59
ATOM	1494	·CZ	PHE	1642	4.705	-0.354	9.855	1.00	28.05
ATOM	1495	C	PHE	1642	7.729	3.139	7.219	1.00	33.35
ATOM ATOM	1496	0	PHE	1642	7.983	3.165	6.018	1.00	36.19
ATOM	1497 1499	N	GLY	1643	6.661	3.746	7.736	1.00	32.76
ATOM	1500	CA C	GLY	1643	5.710	4.419	6.863	1.00	31.44
ATOM	1501	0	GLY	1643 1643	5.805	5.927	6.910	1.00	32.94
ATOM	1501	N	LEU	1644	4.945 6.872	6.636	6.399	1.00	33.10
ATOM	1504	CA	LEU	1644	7.124	6.407	7.525	1.00	35.45
ATOM	1505	CB	LEU	1644	8.387	7.828	7.684	1.00	39.04
ATOM	1506	CG	LEU	1644	8.414	8.011	8.514	1.00	37.80
ATOM	1507	CD1	LEU	1644	7.301	9.120	9.549	1.00	42.51
ATOM	1508	CD2	LEU	1644	9.779	8.887 9.127	10.563	1.00	44.08
ATOM	1509	C	LEU	1644	7.259		10.243 6.357	1.00	44.47
ATOM	1510	Õ	LEU	1644	7.895	8.580 8.107		1.00	42.20
ATOM	1511	N	ALA	1645	6.607	9.732	5.414	1.00	44.14
ATOM	1513	CA	ALA	1645			6.267	1.00	43.89
ATOM	1514	CB	ALA	1645	6.677 5.463	10.569	5.082	1.00	45.62
ATOM	1515	C	ALA	1645		11.493	5.028	1.00	45.06
ATOM	1516	0	ALA	1645	7.966 8.240	11.388	5.186	1.00	45.82
ATOM	1517	N	ARG	1646	8.240 8.766	11.994	6.228	1.00	45.85
ATOM	1519	CA	ARG	1646		11.389	4.129	1.00	45.16
		~~	ARG	7040	10.015	12.140	4.138	1.00	47.06

							14	ŧ U				
	ATOM	1520	CB	ARG	1646							
	ATOM	1521	С		1646	11.	126		318	4.794	1.00	40
	ATOM	1522	0		1646	10.		12.	546	2.742		48.00
	MOTA	1523	· N			10.4		11.		1.823	1.00	46.83
	ATOM	1525	CA		1647	10.8	307	13.		2.578	1.00	45.76
	MOTA	1526	CB		647	11.2	78	14.2		1.288	1.00	48.96
Į		1527	CG	• ~ ~	647	10.9	38	15.7			1.00	50.93
		1528	OD1		647	11.1	91	16.2		1.073	1.00	52.33
A	<b>T</b>	1529	OD2		647	12.2	31	15.8		360	1.00	55.93
		1530			647	10.3		16.9		956	1.00	52.58
		.531	C	ASP 1	647	12.7		10.9	_	.896	1.00	59.54
			0	ASP 1	547	13.49	91	14.1		. 336	1.00	50.78
	_		N	ILE 16	48	13.27	7.4	14.8	03 2		1.00	48.32
					48	14.69	· •	13.1	<b>44</b> 0	~	1.00	50.84
			CB	~	48	14.05		12.83	33 0		1.00	
		536	CG2		48	14.98		11.57	71 -0.	_	1.00	52.58
		537 (	~	ILE 16		14.20		10.38	86 o.	_		50.85
				-0		14.63		11.81		000		49.34
	'OM 15	39 (		_ •		15.23	3 :	10.80		- ·		48.22
AT	OM 15	40				15.52	3 :	13.99			.00	42.86
AT		41 N	. ^	LE 164		16.648		14.22			-00	55.57
AT				IS 164	9	14.944		4.76	- •		.00	57.24
ATO			•	IS 164	9	15.650		5.89		936 1	.00	56.80
ATO				IS 164	9	15.013		6 200		520 1	.00 5	8.03
ATO			•••	IS 164	9	15.221		6.302				8.71
ATC				IS 164	9	16.303		5.308	-	958 1.		0.28
ATO				S 164	9	14.241		4.566		06 1.		0.74
ATO						14.708		4.986				1.70
			E2 HI			15.050	14	4.104	-5.7			
ATO	~ ~ ~ ~		HI		_	15.959	13	8.833	~5.4			1.86
ATO			HI			15.721	17	7.093	-0.5			0.98
ATO		4 N	HI			6.129	18	1.175	-1.0			3.49
ATOM		6 CA			_	5.285	16	.916	0.6			. 56
MOTA		7 CB	HIS		_	5.306	18	.001	1.63			.58
ATOM	1 1558					3.898	18	.540	1.86			.38
ATOM						3.404	19	.433	0.73			.28
ATOM		ND:		-000	1	3.492	20	. 752		_	_	.62
ATOM	1562				1:	2.710	18	. 904	0.53		. •	. 23
ATOM	1563				12	2.402	19	907	-0.33			. 05
ATOM	1565				12	2.863		015	-1.15		0 78	. 51
ATOM	1566		HIS		15	. 925		575	-0.64		0 78.	
ATOM	1567	0	HIS		15	.796		271	2.97		60.	
ATOM	1569	N	ILE	1651		. 584	16.	471	3.969		60.	
ATOM	1570	CA	ILE	1651		.197	16.	419	2.987	1.00	60.	
ATOM		CB	ILE	1651	17	. 574	15.	920	4.204	1.00	60.	03
ATOM	1571	CG2	ILE	1651	1.8	. 280	14.	434	4.069	1.00		
	1572	CG1	ILE	1651	16	.329	13.	920	5.323	1.00		
ATOM	1573	CD1	ILE	1651			13.5	584	3.800			
ATOM	1574	C	ILE	1651	16.	. 635	12.]	124	3.603	1.00		
ATOM	1575	0	ILE		18.	457	16.6	98	4.557			
ATOM	1576	N	ASP	1651	19.	326	16.9	07	3.716	1.00		
ATOM	1578	CA		1652	18.	532	17.1	76	5.793	1.00	59.2	
ATOM	1579	CB	ASP	1652		702	17.9	15		1.00	58.9	
ATOM	1580		ASP	1652	19.		18.7	- J R R	6.260	1.00	58.2	
ATOM	1581	CG	ASP	1652	20.		19.5		7.444	1.00	61.1	
ATOM		OD1	ASP	1652	21.				8.028	1.00	65.3	3
ATOM	1582	OD2	ASP	1652	20.		19.5	/4	7.411	1.00	67.1	
	1583	С	ASP	1652	20.		20.19	_	9.126	1.00	69.04	
CCD1==					-3.	, 50	16.92	22	6.676	1.00	56.75	
JJOU/551	145. v01										50.75	)



ATOM	1584	0	ASP	1652	20.699	16.307	7.741	1.00	56.06	
MOTA	1585	N	TYR	1653	21.794	16.762	5.826	1.00	55.40	
MOTA	1587	CA	TYR	1653	22.900	15.849	6.088	1.00	54.50	
MOTA	1588	CB	TYR	1653	23.825	15.783	4.872	1.00	52.80	
ATOM	1589	CG	TYR	1653	23.334	14.854	3.796	1.00	52.10	
ATOM	1590	CD1	TYR	1653	24.123	14.566	2.685	1.00	51.50	
ATOM	1591	CE1	TYR	1653	23.701	13.658	1.724	1.00	53.52	
ATOM	1592	CD2	TYR	1653	22.099	14.214	3.917	1.00	52.88	
MOTA	1593	CE2	TYR	1653	21.664	13.302	2.966	1.00	54.63	
MOTA	1594	CZ	TYR	1653	22.469	13.025	1.870	1.00	54.35	
MOTA	1595	OH	TYR	1653	22.049	12.107	0.933	1.00	53.23	
ATOM	1597	C	TYR	1653	23.717	16.158	7.339	1.00	55.40	
MOTA	1598	0	TYR	<b>16</b> 53	24.381	15.284	7.900	1.00	54.47	
MOTA	1599	N	TYR	1654	23.673	17.409	7.773	1.00	56.72	
MOTA	1601	CA	TYR	1654	24.421	17.826	8.947	1.00	58.87	
MOTA	1602	CB	TYR	1654	24.978	19.235	8.733	1.00	57.91	
ATOM	1603	CG	TYR	1654	26.068	19.269	7.685	1.00	60.49	
ATOM	1604	CD1	TYR	1654	25.760	19.301	6.325	1.00	61.37	
MOTA	1605	CE1	TYR	1654	26.769	19.289	5.356	1.00	63.72	
MOTA	1606	CD2	TYR	1654	27.412	19.227	8.053	1.00	61.74	
ATOM	1607	CE2	TYR	1654	28.425	19.216	7.099	1.00	64.08	
ATOM	1608	CZ	TYR	1654	28.102	19.248	5.753	1.00	65.12	
ATOM	1609	OH	TYR	1654	29. <b>1</b> 17	19.248	4.817	1.00	64.17	
MOTA	1611	С	TYR	1654	23.628	17.732	10.245	1.00	60.17	
MOTA	1612	0	TYR	1654	24.173	17.935	11.335	1.00	61.09	
MOTA	1613	N	LYS	1655	22.348	17.393	10.133	1.00	60.54	
MOTA	1615	CA	LYS	1655	21.493	17.277	11.306	1.00	62.12	
MOTA	1616	CB	LYS	1655	20.019	17.382	10.910	1.00	64.32	
MOTA	1617	CG	LYS	1655	19.054	17.346	12.079	1.00	67.17	
ATOM	1618	CD	LYS	1655	17.644	17.608	11.602	1.00	73.05	
ATOM	1619	CE	LYS	1655	16.626	17.243	12.660	1.00	77.36	
ATOM	1620	NZ	LYS	1655	15.230	17.494	12.186	1.00	81.10	
ATOM	1624	С	LYS	1655	21.754	15.976	12.057	1.00	62.19	
MOTA	1625	0	LYS	1655	21.902	14.907	11.454	1.00	61.36	
ATOM	1626	N	LYS	1656	21.822	16.084	13.380	1.00	62.26	
ATOM	1628	CA	LYS	1656	22.069	14.933	14.236	1.00	62.28	
ATOM	1629	CB	LYS	1656	23.027	15.310	15.372	1.00	62.05	
ATOM	1630	CG	LYS	1656	24.474	15.489	14.957	1.00	62.62	
ATOM	1631	CD	LYS	1656	25.320	15.889		1.00	66.45	
ATOM	1632	CE	LYS	1656	26.803	15.666	15.908	1.00	67.28	
ATOM ATOM	1633	NZ	LYS	1656	27.619	16.007	17.109	1.00	68.45	
	1637	C	LYS	1656	20.774	14.381	14.824	1.00	61.86	
ATOM	1638	0	LYS	1656	19.714	15.007	14.733	1.00	62.95	
ATOM	1639	N	THR	1657	20.875	13.198	15.420	1.00	60.10	
ATOM	1641	CA	THR	1657	19.743	12.541	16.053	1.00	57.73	
ATOM ATOM	1642	CB	THR	1657	19.973	11.012	16.121	1.00	56.04	
	1643	OG1	THR	1657	21.150	10.730	16.896	1.00	55.21	
MOTA	1645	CG2	THR	1657	20.152	10.431	14.731	1.00	53.07	
ATOM ATOM	1646	C	THR	1657	19.664	13.102	17.472	1.00	57.74	
	1647	0	THR	1657	20.513	13.899	17.870	1.00	57.76	
ATOM	1648	N	THR	1658	18.678	12.667	18.249	1.00	58.80	
ATOM	1650	CA	THR	1658	18.548	13.140	19.627	1.00	60.33	
ATOM	1651	CB	THR	1658	17.318	12.517	20.290	1.00	61.37	
ATOM	1652	С	THR	1658	19.811	12.779	20.406	1.00	60.43	

					172			
ATOM	1653	O THR	7650	<u>.</u> _				
ATOM	1654	N ASN		20.35		99 21	.155 1	00 60
MOTA	<b>-</b>	CA ASN		20.31				.00 60.59
ATOM		CB ASN	1659	21.50	8 11.0			.00 59.97
ATOM		CG ASN	1659	21.60	7 9.5			.00 58.28
ATOM	7.55	DD1 ASN	1659	22.44	8.8			.00 59.95
ATOM			1659	22.382	9.26			.00 60.10
ATOM	1663 C		1659	23.210	7.86			.00 61.26
ATOM	1664 0		1659	22.781	11.71		_	.00 57.09
ATOM	100-	-1014	1659	23.868				00 57.13
ATOM	700-		1660	22.643				00 57.34
ATOM	1667 C		1660	23.781	,	_		00 56.48
ATOM	1668 C	051	1660	24.539	13.27			00 54.87
ATOM	1669 0	$\operatorname{GLY}$	1660	25.716	12.57			
	1670 N	ARG	1661	23.710	12.85		94 1.	
3 00000	1672 CA	ARG	1661	23.879	11.659	9 16.9	18 1.	
	1673 CE		1661	24.536	10.930	15.8		- ,
	1674 CG			24.283	9.428	15.9		
ATOM :	1675 CD		1661	24.848	8.796	17.2		
ATOM	676 NE		1661	24.492	7.325			
	.678 CZ		1661	25.013	6.614			
3.000	679 NH	_	1661	24.902	5.299			
3 770	c		1661	24.286	4.560			
3	685 C		1661	25.426	4.717		-	
3.000			l661	24.076	11.422	19.64		0 47.88
3			1661	23.031	12.029	14.45	9 1.00	9 46.53
3 000		LEU 1	.662	24.839		14.32	5 1.00	45.01
	589 CA	LEU 1	662	24.546	11.094	13.43	2 1.00	42.39
	90 CB	•		25.823	11.503	12.07	5 1.00	
	91 CG	•		26.408	12.031	11.399	1.00	· <del>-</del>
3	92 CD1			27.853	13.332	11.965	1.00	42.44
	93 CD2			25 503	13.478	11.537	1.00	
3 mass	94 C	<del>-</del>		25.591	14.536	11.514	1.00	
ATOM 16	•			23.946	10.362	11.258		
ATOM 16	96 N		_	24.647	9.436	10.862	1.00	38.45
ATOM 16	97 CD		_	2.632	10.428	10.987	1.00	36.67
ATOM 16	98 CA			1.717	11.475	11.489	1.00	37.09
ATOM 16	99 CB		63 2	1.894	9.424	10.207		38.18
ATOM 170				0.535	10 098	9.983	1.00	35.59
ATOM 170			· <del>-</del>	0.343		11.258	1.00	35.90
ATOM 170				2.556	9.045	8.876	1.00	39.13
ATOM 170		PRO 16		2.362	7.933	8.378	1.00	33.05
ATOM 170		VAL 16		3.333	9.960		1.00	31.16
ATOM 170	_	VAL 166		1.020	9.669	8.299	1.00	32.07
ATOM 170		VAL 166	54 24		10.886	7.034	1.00	32.49
3.000		VAL 166	4 23		11 006	6.477	1.00	32.68
	UUL	VAL 166	4 25		11.906	5.864	1.00	32.25
3 0000	_	VAL 166	_	.957	1.523	7.571	1.00	33.22
ATOM 1710	-	VAL 166		.328	8.469	7.171	1.00	29.57
ATOM 1711		LYS 166			7.864	6.175		27.39
ATOM 1713		LYS 166		.303	8.116	8.409		
ATOM 1714		LYS 166			6.991	8.673		28.82
ATOM 1715				.815		0.065		27.87
ATOM 1716				. 967		0.079	_	26.99
ATOM 1717				. 283	_	1.466		29.23
ATOM 1718		LYS 1665		543	^			30.64
ATOM 1722	_	LYS 1665	29.		_			30.94
-122	C I	LYS 1665	25.				1.00	31.63
SSSD/55145. v0				~	υ., ε	3.465		26.76
133145. VC	1							

ATOM	1723	0	LYS	1665	26.211	4.615	8.589	1.00	26.78
ATOM	1724	N	TRP	1666	24.260	5.630	8.137	1.00	25.79
MOTA	1726	CA	TRP	1666	23.561	4.381	7.865	1.00	26.56
MOTA	1727	CB	TRP	1666	22.299	4.273	8.724	1.00	25.63
ATOM	1728	CG	TRP	1666	22.564	3.872	10.174	1.00	26.95
ATOM	1729	CD2	TRP	1666	23.052	4.717	11.232	1.00	24.83
ATOM	1730	CE2	TRP	1666	23.134	3.920	12.398	1.00	24.49
ATOM	1731	CE3	TRP	1666	23.433	6.062	11.306	1.00	24.54
ATOM	1732	CD1	TRP	1666	22.376	2.636	10.730	1.00	20.10
MOTA	1733	NEl	TRP	1666	22.716	2.660	12.063	1.00	21.86
MOTA	1735	CZ2	TRP	1666	23.575	4.433	13.627	1.00	
MOTA	1736	CZ3	TRP	1666	23.870	6.569	12.523	1.00	26.00
MOTA	1737	CH2	TRP	1666	23.939	5.754	13.665	1.00	26.04
ATOM	1738	C	TRP	1666	23.188	4.263	6.386	1.00	23.62
MOTA	1739	0	TRP	1666	22.754	3.214	5.931	1.00	24.87
MOTA	1740	N	MET	1667	23.404	5.330	5.631	1.00	22.78
MOTA	1742	CA	MET	1667	23.046	5.361	4.215	1.00	23.73
ATOM	1743	CB	MET	1667	22.894	6.802	3.744	1.00	26.24
MOTA	1744	CG	MET	1667	21.823	7.621	4.434	1.00	35.55
MOTA	1745	SD	MET	1667	21.795	9.276	3.706	1.00	42.23
ATOM	1746	CE	MET	1667	21.019	8.904	2.238	1.00	40.57
MOTA	1747	С	MET	1667	23.991	4.693	3.239	1.00	22.77
ATOM	1748	0	MET	1667	25.205	4.894	3.294	1.00	24.25
ATOM	1749	N	ALA	1668	23.420	3.963	2.286	1.00	22.73
ATOM	1751	CA	ALA	1668	24.217	3.337	1.237	1.00	23.54
ATOM	1752	CB	ALA	1668	23.339	2.495	0.340	1.00	21.80
MOTA	1753	С	ALA	1668	24.805	4.495	0.430	1.00	25.53
MOTA	1754	0	ALA	1668	24.181	5.551	0.316	1.00	23.66
MOTA	1755	N	PRO	1669	26.006	4.314	-0.153	1.00	26.86
MOTA	1756	CD	PRO	1669	26.899	3.144	-0.095	1.00	26.35
ATOM	1757	CA	PRO	1669	26.611	5.390	-0.942	1.00	27.78
ATOM	1758	CB	PRO	1669	27.864	4.731	-1.518	1.00	25.51
MOTA	1759	CG	PRO	1669	28.225	3.741	-0.471	1.00	25.36
MOTA	1760	С	PRO	1669	25.686	5.900	-2.057	1.00	26.47
MOTA	1761	0	PRO	1669	25.617	7.099	-2.288	1.00	28.42
ATOM	1762	N	GLU	1670	24:951	5.010	-2.724	1.00	26.88
ATOM	1764	CA	GLU	1670	24.057	5.459	-3.796	1.00	29.03
ATOM	1765	CB	GLU	1670	23.597	4.293	-4.693	1.00	31.79
ATOM	1766	CG	GLU	1670	22.588	3.325	-4.065	1.00	32.47
ATOM	1767	CD	GLU	1670	23.212	2.184	-3.255	1.00	32.43
MOTA	1768	OE1	GLU	1670	22,429	1.297	-2.822	1.00	25.01
MOTA	1769	OE2	GLU	1670	24.458	2.157	-3.069	1.00	28.75
ATOM	1770	С	GLU	1670	22.864	6.274	-3.294	1.00	28.37
ATOM	1771	0	GLU	1670	22.358	7.146	-4.001	1.00	25.72
ATOM	1772	N	ALA	1671	22.451	6.028	-2.053	1.00	30.08
MOTA	1774	CA	ALA	1671	21.347	6.779	-1.465	1.00	31.24
ATOM	1775	CB	ALA	1671	20.751	6.031	-0.287	1.00	26.42
ATOM	1776	C	ALA	1671	21.899	8.125	-1.013	1.00	31.36
ATOM	1777	0	ALA	1671	21.298	9.167	-1.249	1.00	33.11
ATOM	1778	N	LEU	1672	23.068	8.096	-0.387	1.00	32.73
ATOM	1780	CA	LEU	1672	23.715	9.304	0.100	1.00	33.96
ATOM	1781	CB	LEU	1672	24.931	8.935	0.940	1.00	33.89
ATOM	1782	CG	LEU	1672	25.783	10.071	1.502	1.00	37.62
ATOM	1783	CD1	LEU	1672	25.010	10.800	2.581	1.00	39.57



		784 C	D2 L	EU 1672	27.054	• • •	_		
		785 C		EU 1672					32.30
		786 O		_				-	
		'87 N	PF						37.87
		'89 C	A PH				-		
		90 C	в рн		-4.100				35.82
AT			G PH		-0.,50	9.802	·		34.66
AT		92 CI	D1 PH			9.642			33.84
AT		93 CI	02 PH		28.242	8.422		1.00	32.65
ATO		94 CE	El PH		29.540	=0.703		1.00	36.98
ATO		95 CE	2 PH		29.279	8.257		1.00	37.95
ATO		96 CZ	PH		29.927	10.557		1.00	39.90
ATO		97 C	PHI		24.483	9.325		1.00	37.09
ATC		-	PHI		24.430	10.692		1.00	36.34
ATC		99 N	ASI		23.705	11.788	_	1.00	37.18
ATO		1 CA	ASI		22.780	9.677		1.00	38.22
ATO		2 CB	ASI		23.008	9.777	-5.693	1.00	38.51
ATO		3 CG	ASF		24.439	8.597	-6.633	1.00	40.34
ATO		4 OD:	1 ASP		25.092	8.511	-7.122	1.00	43.87
ATO			2 ASP		24.906	9.571	-7.254	1.00	42.79
ATO		_	ASP		21.298	7.376	-7.369	1.00	47.94
ATO			ASP		20.457	9.853	-5.360	1.00	40.21
ATO			ARG	1675	20.975	9.872	-6.271	1.00	39.07
ATO			ARG	1675	19.589	9.836	-4.072	1.00	39.83
ATON			ARG	1675	18.992	9.900 11.271	-3.631	1.00	42.25
ATON	<b>-</b> -		ARG	1675	19.691	12.420	-3.964	1.00	48.19
ATOM			ARG	1675	19.462	13.729	-3.267	1.00	59.20
ATOM			ARG	1675	20.079	14.876	-4.019	1.00	67.81
ATOM			ARG	1675	19.688	16.136	-3.352	1.00	75.11
ATOM ATOM			ARG	1675	18.680	16.429	-3.525 -4.341	1.00	78.74
ATOM			ARG	1675	20.311	17.115	-2.890	1.00	79.91
ATOM		-	ARG	1675	18.730	8.777	-4.221		81.24
ATOM		-	ARG	1675	17.544	8.956			39.00
ATOM			ILE	1676	19.345	7.624			39.71
ATOM	,	CA	ILE	1676	18.636	6.471			35.50
ATOM	1829	CB	ILE	1676	19.434	5.759			33.51
ATOM	1830	CG2	ILE	1676	18.582	4.678	<b>.</b>		34.59
ATOM	1831	CG1 CD1	ILE	1676	19.848	6.752			33.90 37.60
ATOM	1832	CDI	ILE	1676	20.861	6.197			12.67
ATOM	1833	0	ILE	1676	18.390	5.501			30.94
ATOM	1834	N	ILE	1676	19.326	4.926			8.62
ATOM	1836	CA	TYR	1677	17.124	5.351			0.60
ATOM	1837	CB	TYR	1677	16.724	4.467			5.87
ATOM	1838	CG	TYR	1677	15.781				6.40
ATOM	1839	CD1	TYR	1677	16.483				7.67
ATOM	1840	CE1	TYR	1677	16.663	~			7.45
ATOM	1841	CD2	TYR	1677	17.269			_	6.55
ATOM	1842	CE2	TYR		16.935	5.883			4.58
ATOM	1843	CZ	TYR		17.536	6.828			6.35
ATOM	1844	OH			17.698	8.122			3.80
ATOM	1846	C	_		18.270	9.059	_		1.97
ATOM	1847	0			16.055	3.235 -			2.70
ATOM	1848	N			15.144	3.335 -			5.22
		44	THR	1678	16.477		_		L.83

					113					
					050	0.791	-2.865	1.00	22.14	
» IDOM	1850	CA	THR	1678	15.968	0.191	-3.928	1.00	23.91	
MOTA	1851	CB	THR	1678	16.907	0.105	-3.373	1.00	27.47	
ATOM	1852	OG1	THR	1678	18.229	1.053	-5.188	1.00	24.94	
MOTA MOTA	1854	CG2	THR	1678	16.949	-0.176	-1.692	1.00	22.7	
	1855	С	THR	1678	15.999	0.170	-0.592	1.00	23.3	
MOTA MOTA	1856	0	THR	1678	16.427	-1.402	-1.929	1.00	21.9	
ATOM	1857	N	HIS	1679	15.563 15.613	-2.417	-0.888	1.00	22.9	
MOTA	1859	CA	HIS	1679	14.872	-3.671	-1.351	1.00	22.0	44 1
ATOM	1860	CB	HIS	1679	13.421	-3.444	-1.621	1.00	25.4	
ATOM	1861	CG	HIS	1679	12.674	-3.611	-2.740	1.00		
MOTA	1862	CD2	HIS	1679	12.556	-2.954	-0.663	1.00		
MOTA	1863	ND1	HIS	1679	11.348	-2.830	-1.178	1.00		
MOTA		CEl	HIS	1679	11.394	-3.221	-2.441			
ATOM			HIS	1679	17.097	-2.719	-0.650			
ATOM			HIS	1679	17.537	-3.074	0.459			
ATOM	0	_	HIS		17.895	-2.506	-1.697			30 33
ATOM			GLN		19.335	-2.726	-1.658			50
ATOM			GLN		19.948	-2.594	-3.05			15
ATON			GLN		19.895	-3.872	-3.87			
OTA		4 CG	GL1		18.865	-3.847	-4.99	1 1.0		.43
ATO		5 CD	GL1		17.819	-3.212	2 -4.87	1 1.0		.44
ATO		6 OE:				-4.54	2 -6.08	5 1.0		.61
ATO						-1.74	0 -0.73			.00
ATO		0 C	GL		043	-2.09	3 -0.02			.06
OTA		1 0	GL		-0 500	-0.49				.41
ATO			SE		101	0.47				.06
ATC						1.92	3 -0.30			.90
ATO					-0 -02	2.16	6 -0.4		00 23	3.08
ATC					770	0.20		-	00 24	1.13
TA	OM 18				20, 236	0.53				3.19
TA	OM 18		_			3 -0.43				2.37
AT	OM 18		_		10'	7 -0.7		-	00 2	4.55
TA		_				0 -1.2	75 3.0	_	.00 2	4.22
AT		-	_	SP 168 SP 168		6 -0.1			.00 2	5.02
ΓA			_	SP 168	14.42	B -0.4		. • -		4.82
FA	-			SP 168	15.94	9 0.9	<del>-</del> -			0.47
A7				SP 16	82 18.98	0 -1.8				21.83
A.			_	ASP 16	82 19.17					20.14
			٠.	VAL 16	83 19.48	30 -2.			.00	20.49
				VAL 16	83 20.34	10 -3.		003	.00	22.38
					83 20.45	93 -4.			1.00	19.57
					83 21.7	57 -5.	_		1.00	22.35
			_		83 19.2	• -			1.00	20.22
			•		83 21.6				1.00	21.41
_		1905	C		583 22.2			-	1.00	21.33
		1906	O N		684 22.2		_		1.00	22.21
		1907	N CA		684 23.4			.540	1.00	18.78
		1909	CA		684 23.7			.037	1.00	22.80
		1910	CB		684 24.5			.472	1.00	24.60
		1911	CC		684 26.3		• -	.286	1.00	24.34
		1912	CD2 CE2		684 26.			.352	1.00	24.32
-	MOTA	1913		4	684 26.			1.138	1.00	22.28
	ATOM	1914	CE3		L684 24.	933 1	.208 4			
	MOTA	1915								

	_						_	146					
	ATOM	1916	NE1	TRP	1.00.								
	ATOM	1918		TRP	1684	-0	.169		1.791	1	202		
	ATOM	1919		TRP	1684	28.	324		1.669		297	1.00	22.32
	ATOM	1920	CH2		1684	28.	193		0.213		022	1.00	24.77
	ATOM	1921	C	TRP	1684	28.	906		.088		090	1.00	24.46
	ATOM	1922	o	TRP	1684	23.	198	- 1	.183		918	1.00	24.00
	ATOM	1923		TRP	1684	23.	982				899	1.00	23.26
	ATOM	1925	N ~-	SER	1685	22.	108		.475	5.8	805	1.00	24.52
	ATOM		CA	SER	1685	21	744		.447	5.3	113	1.00	
	ATOM	1926	CB	SER	1685	20.3	,44		.057	6.4		1.00	22.88
	ATOM	1927	OG	SER	1685	20.2	98		. 783	6.3		1.00	24.01
	> ma	1929	C	SER	1685	20.4	24	1.	787	5.3		1.00	21.90
	•	1930	0	SER	1685	21.6	59	-1.	087	7.4		1.00	24.75
		1931	N	D	1686	22.0	77	-0.	933	8.6		1.00	24.28
	MOTA	1933	CA	B		21.0	99	-2.	221	7.0		1.00	23.94
	MOTA	1934	~-		1686	20.9	93	-3.	393			1.00	23.20
	TOM 1	1935	_		1686	20.2	16	-4.	 519	7.89		1.00	23.87
A	TOM 1	936	~	-	686	20.08	52	-5.	724	7.21		1.00	19.56
A	mo.		~		.686	19.24	10	-5.1	7.34	8.07			22.19
A	·			PHE 1	686	20.77	73	· J .	, O.T	9.20	3 1		21.55
	_		<b>~</b>		686	19.12	5	-6.8		7.79	3 1		21.94
A:	71000	<b>~</b>		HE 1	686	20.66		-6.8		0.03	3 1		1.66
		_		PHE 1	686	19.84		-8.0	12	8.62		-	2 47
					586	22.38		-7.9	61	9.74			2.47
		942 (	-		86	22 - 20		-3.8	90 (	8.300			3.14
		43 N	Ţ G			22.579		-4.4	24 9	9.407		_	2.62
		45 C	'A G			23.354		3.72		7.401		-	3.09
AT		46 C			_	24.718	} -	4.11		7.721		00 2	3.50
AT		47 0				<sup>25</sup> .230	-	3.24		.867		00 23	3.83
ATO						25.901	-	3.74		7.778			. 95
ATO		50 C		_	_	24.928	~	1.94				00 23	. 76
ATC			***			25.331	-	1.00		.817	1.	00 20	.60
ATC	M 19 <u>5</u>	52 CG	***	_	_	5.020		0.48		.877	1.0	00 22	.34
ATO		3 CG			88 2	5.547		1.43		488	1.0	00 20	. 94
ATO	M 195				_	5.675		0.832		. 543	1.0	00 21	. 65
ATO	M 195	_	VAI		8 2	4.598	~ 7	400		160	1.0	0 22	. 71
ATO	M 195	_	IAV		8 2	5.199	. 7	.400		182	1.0	0 22.	71
ATO		_	LEU		9 2:	3.310	-1	.479		255	1.0		70
ATON	1 195		LEU	168	9 25	2.534		. 706	_	082	1.0	0 22.	70
ATOM			LEU	168	9 21	.064		.111	- •	253	1.0		
ATOM			LEU	1689	_	0.004		.357	11.	866	1.0		
ATOM				1689				. 491	12.9		1.00		
ATOM	-502		LEU	1689		.643		109	12.4	108	1.00		18
			LEU	1689		. 959		895	13.5	553	1.00	•	
ATOM			LEU	1689		.158	-3.	375	12.8				77
ATOM	1965	N	LEU	1690		. 249	-3.	483	14.0		1.00	_	88
ATOM	1967	CA	LEU			. 588	-4.	323	12.0		1.00		
ATOM	1968	CB	LEU	1690	24.	.221	-5.	544			1.00		
ATOM	1969	CG	LEU	1690	24.	669	-6.	444	12.5		1.00	24.4	3
ATOM	1970	CD1		1690	23.	672	-7.3	300	11.3		1.00	26.3	
ATOM	1971	CD2	LEU	1690	24.	415	-7.9	367	10.60		1.00	26.5	
MOTA	1972	C C	LEU	1690	23.	042	-8.3	100	9.44		.00	26.3	3
ATOM	1973		LEU	1690	25.	430		.00	11.50	)2 1	00	24.66	
ATOM	1974	0	LEU	1690	25.	646	-5.1	.08	13.34	9 1	.00	25.22	
ATOM		N	TRP	1691	26.2	211	-5.7	06	14.43	5 1	.00	24.84	•
ATOM	1976	CA	TRP	1691	27.4		-4.2		12.82	_	.00	25.04	
ATOM	1977	CB	TRP	1691	20 -		-3.7		13.50		.00	26.92	
AT OM	1978	CG		1691	28.0		-2.6	59	12.63	_	.00	25.77	
66cv :-	_				29.3	94	-2.19	95	13.154		.00	24.82	
SSSD/55	145. v01									- 1.	. 00	27.98	

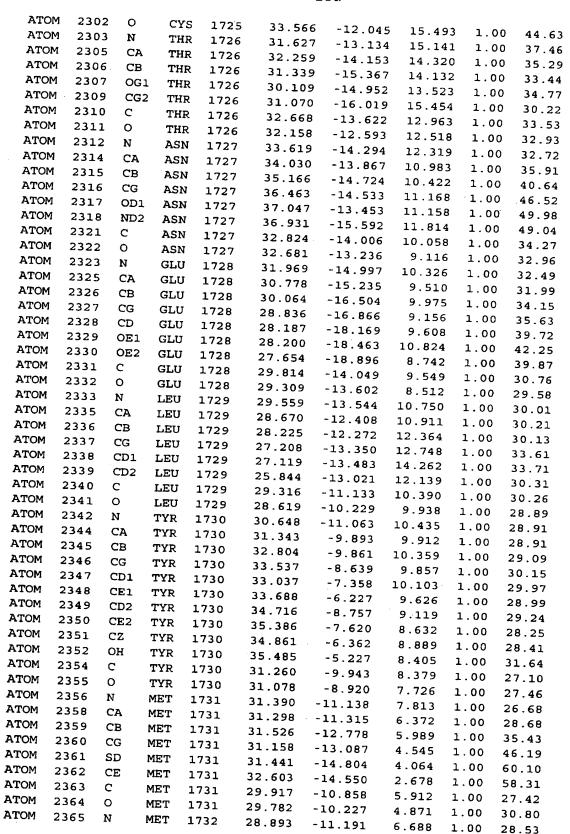
MOTA 1979 CD2 TRP 1691 29.623 -1.104 14.056 1.00 26.95 MOTA 1980 CE2 TRP 1691 31.022 -1.015 14.259 1.00 27.64 MOTA 1981 CE3 TRP 1691 28.783 -0.191 14.708 1.00 MOTA 1982 CD1 TRP 1691 30.634 -2.715 12.856 1.00 28.38 MOTA 1983 NE1 TRP 1691 31.609 -2.009 13.518 1.00 29.56 ATOM 1985 CZ2 31.599 -0.045 TRP 1691 15.086 1.00 27.78 29.356 0.769 ATOM 1986 CZ3 TRP 1691 15.533 1.00 27.63 ATOM 1987 CH2 TRP 30.753 1691 0.835 15.713 1.00 30.68 MOTA 1988 C TRP 1691 27.025 -3.147 14.876 1.00 26.38 MOTA 1989 0 TRP 1691 27.686 -3.414 15.883 1.00 24.82 MOTA 1990 N GLU 1692 25.926 -2.393 14.916 1.00 27.62 MOTA 1992 CA GLU 1692 25.442 -1.790 16.162 1.00 27.02 MOTA 1993 CB 15.919 GLU 1692 24.193 -0.963 1.00 29.27 ATOM 1994 CG GLU 24.345 1692 0.236 15.028 1.00 24.77 MOTA 1995 CD GLU 1692 23.046 0.992 14.962 1.00 25.98 ATOM 1996 OE1 GLU 1692 22.238 0.694 14.058 1.00 22.29 **ATOM** 1.837 1997 OE2 GLU 1692 22.803 15.850 1.00 25.12 1998 MOTA C GLU 1692 25.092 -2.856 1.00 17.191 27.88 MOTA 1999 0 GLU 1692 25.333 -2.673 18.379 1.00 30.18 MOTA 2000 N ILE 1693 24.500 -3.956 16.734 1.00 26.65 MOTA 2002 CA ILE 1693 24.118 -5.054 17.618 1.00 26.14 ATOM 2003 CB ILE 1693 23.279 -6.144 16.858 1.00 25.37 MOTA 2004 CG2 ILE 1693 23.144 -7.445 17.704 1.00 21.48 MOTA 2005 CG1 ILE 1693 21.897 -5.563 16.496 1.00 24.80 MOTA 2006 CD1 ILE 1693 21.017 -6.479 15.642 1.00 22.40 ILE **ATOM** 2007 С 1693 25.345 -5.698 18.239 1.00 27.17 MOTA 2008 C ILE 1693 25.424 -5.864 19.452 1.00 27.30 MOTA 2009 N PHE 1694 26.329 -6.017 17.414 1.00 29.98 MOTA 2011 CA PHE 1694 27.518 -6.674 17.925 30.61 1.00 MOTA 2012 CB PHE 1694 -7.556 28.140 16.843 1.00 28.30 MOTA 2013 CG PHE 1694 27.197 -8.611 16.353 1.00 30.91 MOTA 2014 CD1 PHE 1694 26.627 -8.526 15.088 1.00 34.46 MOTA 1.00 2015 CD2 PHE 1694 17.224 26.743 -9.601 32.71 MOTA 2016 CEl PHE 1694 25.622 -9.409 14.701 1.00 34.24 MOTA 2017 CE2 PHE 1694 25.737 -10.490 16.844 1.00 32.44 ATOM 2018 CZPHE 1694 25.170 1.00 -10.387 15.592 32.70 ATOM 2019 С PHE 1694 28.512 -5.796 18.689 1.00 31.74 ATOM 2020 0 PHE 1694 -6.299 29.469 19.276 1.00 35.15 MOTA 2021 THR N 1695 28.275 -4.489 18.698 1.00 31.12 MOTA 2023 CA THR 1695 29.101 -3.575 19.473 1.00 29.96 MOTA 2024 CB THR 1695 29.532 -2.351 18.657 1.00 28.09 ATOM 2025 OG1 THR 1695 28.373 -1.685 18.150 1.00 30.65 MOTA 2027 CG2 THR 1695 30.450 -2.767 17.510 1.00 23.37 MOTA 2028 С THR 1695 28.240 -3.128 20.664 1.00 30.01 MOTA 2029 -2.233 0 THR 1695 28.617 21.427 1.00 31.14 MOTA 2030 N LEU 1696 27.078 -3.766 20.797 1.00 27.96 MOTA 2032 CA LEU 1696 26.113 -3.490 21.862 1.00 30.25 MOTA 2033 CB LEU 1696 26.633 -3.985 23.216 1.00 33.54 MOTA 2034 CG LEU 1696 26.899 -5.482 23.339 1.00 32.61 MOTA 2035 CD1 LEU 1696 27.473 -5.777 24.711 1.00 33.54 MOTA 2036 CD2 LEU 1696 25.602 -6.233 23.126 1.00 36.37 MOTA 2037 С LEU 1696 25.717 -2.031 21.958 1.00 28.19 MOTA 2038 LEU 0 1696 25.792 -1.431 23.018 1.00 29.18 MOTA 2039 N GLY 1697 25.251 -1.472 20.853 1.00 28.24

	ATOM	2041	CA	GTV	1						
	ATOM	2042	C.	~	1697	24.		-0.082	20.858		
	ATOM	2043	ō		1697	25.	990	0.845	20.499	1.00	28.29
	ATOM	2044	N	~	1697	25.		2.022	20.846	1.00	27.68
	ATOM	2046	CA		1698	26.9		_	19.790	1.00	29.79
	ATOM	2047	C		698	28.1		_		1.00	29.23
	ATOM	2048	o ·	~	698	27.7	43		19.396	1.00	30.79
	ATOM	2049	N		698	26.8	17	_	18.388	1.00	32.38
	3 63 6 4 4	2051	CA		699	28.4	_	_	17.601	1.00	33.26
ž		2052	CB		699	28.2	68 <sub>4</sub>	_	18.411	1.00	30.81
1		2053	OG		699	28.5	ءِ 28			1.00	32.03
7		2055	C		599	28.5				1.00	34.81
7		2056	0		599	29.19	98 4	_	7.440	1.00	40.03
A	ma	057			99	30.42				1.00	32.20
	ma	058	<b>~</b>		00	28.62	_			1.00	31.67
A					00	27.17	_			1.00 ;	32.62
				PRO 17	00	29.42	_		4.773 ]		4.19
			~~	PRO 17	00	28.35	_		3.856 1		1.76
			_	PRO 17	00	27.14		_	2.759 <sub>l</sub>		2.04
			~	PRO 17	00	30.21		351 13	1.502 1		3.17
	30	٠		PRO 170	00	29.715		309 13	.609 1		8.70
			•	YR 170	) 1	31.459	- •	391 13	.871 1		8.57
				YR 170	1	32.311	- •	181 13	.164 1		3.61
AT				YR 170		31.920		338 12	.870 1.		9.92
AT	^			YR 170	1	31.965	-		.510 1.	_	).15
AT		~ ~		YR 170	1	30.799			.339 1.		.17
ATO				YR 170	1 :	30.839			664 1.	_	.26
ATO				(R 170		33.176				_	.51
ATO			E2 TY			33.229	5.4		893 1.	^ -	.48
ATO			Z TY			32.059	4.6	07 8.	805 1.	_	. 48 . 94
ATO		•	TY.		_	32.110	4.2		146 1.		. 72
		_	TY		_	2 220	3.4	31 7.	043 1.0	_	
ATO ATO		_	TY		_	2.279	7.4	48 13.	941 1.0		
		- 4.	PR		_	1.935	8.5	92 13.6			
ATO	,		PRO			2.649	7.1	35 15.3			
ATO			PRO		3.	3.212	5.87	79 15.7	708 1.0		66
ATON			PRO		J.	2.631	8.17	<sup>73</sup> 16.2	31 1.0		83
ATOM	-002		PRO			3.116	7.43	2 17.4	79 1.0		54
ATOM		_	PRO			2.903	6.00	1 17.1			TR
ATOM	-009	0	PRO		33	3.628	9.27	4 15.8			
ATOM			GLY		34	.750	8.98	1 15.4			
ATOM		CA	GLY		3.3	.220	10.52	B 16.0	74 1.00		
ATOM		C	GLY	1703	34	. 085	11.66	7 15.74	38 1.00		5
MOTA	2089	0	GLY	1703	34	.245	12.006	5 14.31	1.00		
ATOM	2090	N	VAL	1704	34	. 977	12.933	13.96			
MOTA	2092	CA	VAL	1704	33	. 552	11.275	13.44			
ATOM	2093	CB	VAL		33.	.641	11.512	12.00	_	- ·	
ATOM	2094	CG1	VAL	1704	33.	614	10.176	11.22			
ATOM	2095	CG2	VAL	1704	33.	628	10.435		-	31.3	
ATOM	2096	C	VAL	1704	34.	796	9.297		•	31.46	
ATOM	2097	ō		1704	32.	510	12.410	11.51		27.62	
ATOM	2098	N	VAL	1704	31.	337	12.070	11.64		33.35	
ATOM	2099	CD	PRO	1705	32.	849	13.589			33.94	
ATOM	2100	CA	PRO	1705	34.	181	14.221	10.974		32.43	
ATOM	2101	CB	PRO	1705	31.	826	14.505	10.949		32.77	
		CB	PRO	1705	32.5	_	15.853	10.472		33.61	
SSSD/55	145. v01					·		10.509	1.00	33.21	

MOTA	2102	CG	PRO	1705	33.935	15.482	10.141	1.00	35.53
MOTA	2103	С	PRO	1705	31.395	14.138	9.052	1.00	33.91
MOTA	2104	0	PRO	1705	32.113	13.409	8.354	1.00	32.65
ATOM	2105	N	VAL	1706	30.255	14.684	8.619	1.00	33.82
ATOM	2107	CA	VAL	1706	29.689	14.447	7.280	1.00	33.97
MOTA	2108	СВ	VAL	1706	28.617	15.513	6.943	1.00	37.41
ATOM	2109	CG1	VAL	1706	28.045	15.282	5.556	1.00	41.12
ATOM	2110	CG2	VAL	1706	27.507	15.484	7.971	1.00	38.89
ATOM	2111	С	VAL	1706	30.712	14.428	6.135	1.00	32.32
ATOM	2112	0	VAL	1706	30.819	13.450	5.398	1.00	32.58
ATOM	2113	N	GLU	1707	31.477	15.504	6.004	1.00	31.15
ATOM	2115	CA	GLU	1707	32.478	15.630	4.956	1.00	29.82
ATOM	2116	СВ	GLU	1707	33.172	16.989	5.048	1.00	30.05
ATOM	2117	C	GLU	1707	33.531	14.541	4.959	1.00	28.52
ATOM	2118	ō	GLU	1707	33.995	14.134	3.896	1.00	30.85
ATOM	2119	N	GLU	1708	33.958	14.110	6.143	1.00	28.70
ATOM	2121	CA	GLU	1708	34.978	13.073	6.235	1.00	29.50
ATOM	2122	CB	GLU	1708	35.590	13.073	7.641	1.00	31.28
ATOM	2123	CG	GLU	1708	36.281	14.289	8.103	1.00	41.63
ATOM	2124	CD	GLU	1708	37.454	14.718	7.237	1.00	49.91
ATOM	2125	OE1	GLU	1708	38.020	13.876	6.498	1.00	53.57
ATOM	2126	OE2	GLU	1708	37.821	15.916	7.308	1.00	58.45
ATOM	2127	C	GLU	1708	34.365	11.730	5.878	1.00	30.00
MOTA	2128	0	GLU	1708	35.016	10.874	5.257	1.00	
ATOM	2129	N	LEU	1708	33.103	11.559	6.257	1.00	28.43 30.08
ATOM	2131	CA	LEU	1709	32.392	10.324	5.964	1.00	29.19
ATOM	2132	CB	LEU	1709	30.995	10.347	6.592	1.00	28.97
ATOM	2133	CG	LEU	1709	30.109	9.186	6.137	1.00	30.66
ATOM	2134	CD1	LEU	1709	30.664	7.866	6.659	1.00	29.24
MOTA	2135	CD2	LEU	1709	28.684	9.403	6.593	1.00	29.29
ATOM	2136	C	LEU	1709	32.294	10.130	4.449	1.00	28.26
ATOM	2137	0	LEU	1709	32.450	9.011	3.948	1.00	28.86
ATOM	2138	N	PHE	1710	32.430	11.220	3.735	1.00	26.86
ATOM	2140	CA	PHE	1710	31.903	11.192	2.285	1.00	28.86
ATOM	2141	CB	PHE	1710	31.632	12.593	1.743	1.00	31.88
ATOM	2142	CG	PHE	1710	30.249	13.095	2.014	1.00	37.62
ATOM	2143	CD1	PHE	1710	29.265	12.247	2.509	1.00	42.63
ATOM	2144	CD2	PHE	1710	29.931	14.424	1.792	1.00	43.53
ATOM	2145	CE1	PHE	1710	27.977	12.718	2.783	1.00	45.99
ATOM	2146	CE2	PHE	1710	28.648	14.905	2.061	1.00	46.25
ATOM	2147	CZ	PHE	1710	27.670	14.045	2.559	1.00	44.45
ATOM	2148	C	PHE	1710	33.193	10.660	1.681	1.00	30.42
ATOM	2149	ο .	PHE	1710	33.174	9.807	0.792	1.00	29.01
ATOM	2150	N	LYS	1711	34.309	11.152	2.212	1.00	30.64
ATOM	2152	CA	LYS	1711	35.650	10.762	1.786	1.00	32.89
MOTA	2153	CB	LYS	1711	36.670	11.655	2.502	1.00	
ATOM	2154	CG	LYS	1711			2.088		37.91
ATOM	2155	CD	LYS	1711	38.108 38.976	11.479 12.528		1.00	42.99
ATOM	2156	CE				12.528	2.752	1.00	47.45
ATOM	2156	NZ	LYS	1711	40.380	12.505	2.182	1.00	52.35
ATOM	2157	NZ C	LYS	1711	41.104	11.272	2.587	1.00	58.47
ATOM	2161		LYS	1711	35.913	9.273	2.071	1.00	32.23
ATOM		ν. Ο	LYS	1711	36.445	8.559	1.216	1.00	30.79
ATOM	2163	N	LEU	1712	35.533	8.807	3.264	1.00	31.37
ATOM	2165	CA	LEU	1712	35.704	7.399	3.630	1.00	29.46

2	77014									
		2166	CB	LEU 1	712	35.22	20 7 -			
		2167	CG		712	36.04			065 1	.00 28.57
			CD1		712				242 1	.00 30.18
A.	TOM 2	169			712	35.39	_		569 1	.00 26.92
	rom 2	170	_	_	712	37.45				.00 30.88
A7	rom 2			_		34.92				
A					712	35.43				
					713	33.67	5 6.9			00 30.73
					713	32.85				00 30.13
				EU 17	713	31.413			-·	00 32.10
				EU 17	713	30.612				00 35.23
			D1 L	EU 17	13	29.265		_		00 37.47
AT			D2 L		13	30.447				00 40.85
AT		.79 C	L		13				23 1.	00 39.61
ATO	OM 21	80 C		EU 17		33.441			47 1.	
ATO	OM 21	81 N				33.548		0 -0.5		•
ATO	OM 21					33.859		9 -0.4		
ATO		_				34.440	7.38		٠	2
ATO		_				34.826	8.82			50
ATC					14	33.640	9.73			
ATO			_			32.736	9.23			
ATO				'S 171		31.635	10.24			
			Z Ly	S 171		30.727		-		
ATO			LY			35.664	9.80			0 47.40
ATO		-	LY			35.927	6.488			
ATO		4 N	GL				5.898		7 1.0	0 36.68
ATO		6 CA				36.376	6.338			
ATO		7 CB				37.577	5.527		9 1.00	
ATON	M 219	8 CG				8.566	6.125	0.25		
ATOM	1 219					8.967	7.537	-0.163		
ATOM	1 220				_	9.735	8.310	0.893		
ATOM						9.906	7.814			,5
ATOM						0.163	9.442	0.572		
ATOM			GLU		_	7.321	4.048	-0.487		
ATOM			GLU		3	8.259	3.260			
ATOM			GLY			6.049	3.674	-0.438		· - <del>-</del>
ATOM	0		GLY	1716		5.695	2.288	-0.366		
	,	_	GLY	1716		5.966		-0.133		27.58
ATOM		-	GLY	1716		5.069	1.765	1.262	1.00	28.60
ATOM		N	HIS	1717		.062	0.560	1.464	1.00	27.81
ATOM	2211	CA	HIS	1717		3.319	2.663	2.236	1.00	29.10
ATOM	2212	CB	HIS	1717			2.263	3.617	1.00	29.30
ATOM	2213	CG	HIS	1717		.501	3.510	4.486	1.00	30.54
ATOM	2214	CD2	HIS			.788	3.213	5.930	1.00	32.88
ATOM	2215	ND1	HIS	1717		.961	3.023	6.586	1.00	32.21
ATOM	2217	CE1		1717	35	.798	3.108	6.881	1.00	
ATOM	2218	NE2	HIS	1717	36	.342	2.865	8.061	1.00	34.22
ATOM	2220		HIS	1717	37	.651	2.809	7.907		31.51
ATOM		C	HIS	1717		.180	1.416		1.00	31.94
ATOM	2221	0	HIS	1717		.017	1.666	4.183	1.00	28.42
	2222	N	ARG	1718		. 526		3.885	1.00	30.71
ATOM	2224	CA	ARG	1718		. 559	0.450	5.028	1.00	27.75
ATOM	2225	CB	ARG	1718		562	-0.423	5.688	1.00	27.58
ATOM	2226	CG	ARG	1718			-1.813	5.048	1.00	29.07
MOTA	2227	CD	ARG	1718		078	-1.860	3.597	1.00	28.39
ATOM	2228	NE	ARG			609	-1.412	3.475	1.00	27.64
ATOM	2230	CZ		1718	32.	091	-1.467	2.096	1.00	
ATOM	2231	NH1	ARG	1718	32.	173	-0.476	1.210	1.00	24.37
		TALIT	ARG	1718	32.	768	0.668	1.532		24.26
SSSD/ss	146							~2	1.00	23.98

ATOM	2234	NH2	ARG	1718	31.595	-0.603	0.019	1.00	21.60
MOTA	2237	С	ARG	1718	35.005	-0.521	7.148	1.00	30.11
MOTA	2238	0	ARG	1718	36.201	-0.623	7.428	1.00	30.60
MOTA	2239	N	MET	1719	34.056	-0.430	8.074	1.00	30.69
ATOM	2241	CA	MET	1719	34.350	-0.490	9.501	1.00	31.77
ATOM	2242	CB	MET	1719	33.072	-0.302	10.335	1.00	34.56
ATOM	2243	CG	MET	1719	32.408	1.060	10.194	1.00	36.71
MOTA	2244	SD	MET	1719	31.015	1.307	11.314	1.00	38.66
ATOM	2245	CE	MET	1719	29.797	0.338	10.544	1.00	36. <b>9</b> 9
ATOM	2246	С	MET	1719	34.998	-1.810	9.854	1.00	30.20
MOTA	2247	0	MET	1719	34.802	-2.802	9.169	1.00	31.41
MOTA	2248	N	ASP	1720	35.778	-1.809	10.926	1.00	32.49
MOTA	2250	CA	ASP	1720	36.473	-3.008	11.385	1.00	33.60
MOTA	2251	CB	ASP	1720	37.593	-2.630	12.358	1.00	37.65
ATOM	2252	CG	ASP	1720	38.628	-1.688	11.747	1.00	44.69
ATOM	2253	OD1	ASP	1720	38.442	-1.223	10.596	1.00	50.97
MOTA	2254	OD2	ASP	1720	39.632	-1.398	12.443	1.00	48.67
MOTA	2255	С	ASP	1720	35.524	-3.977	12.079	1.00	31.26
ATOM	2256	0	ASP	1720	34.466	-3.581	12.561	1.00	32.69
ATOM	2257	N	LYS	1721	35.943	-5.231	12.191	1.00	32.76
MOTA	2259	CA	LYS	1721	35.133	-6.261	12.825	1.00	32.28
MOTA	2260	CB	LYS	1721	35.726	-7.649	12.575	1.00	33.63
MOTA	2261	CG	LYS	1721	34.854	-8.773	13.125	1.00	35.68
ATOM	2262	CD	LYS	1721	35.392	-10.126	12.784	1.00	36.22
ATOM	2263	CE	LYS	1721	36.054	-10.749	13.988	1.00	42.65
ATOM	2264	NZ	LYS	1721	36.354	-12.189	13.756	1.00	46.15
ATOM	2268	С	LYS	1721	35.039	-6.051	14.315	1.00	35.55
ATOM	2269	0	LYS	1721	36.064	-5.926	14.986	1.00	37.78
ATOM	2270	N	PRO	1722	33.807	-6.017	14.861	1.00	36.91
ATOM	2271	CD	PRO	1722	32.504	-6.105	14.179	1.00	34.43
ATOM	2272	CA	PRO	1722	33.630	-5.827	16.305	1.00	37.77
ATOM	2273	CB	PRO	1722	32.107	-5.846	16.465	1.00	36.32
ATOM	2274	CG	PRO	1722	31.603	-5.375	15.122	1.00	34.53
ATOM	2275	C	PRO	1722	34.246	-7.026	17.023	1.00	39.31
ATOM	2276	0	PRO	1722	34.274	-8.136	16.477	1.00	38.78
ATOM	2277	N	SER	1723	34.777	-6.820	18.222	1.00	42.72
ATOM ATOM	2279	CA	SER	1723	35.336	-7.954	18.940	1.00	45.01
ATOM	2280 2281	CB OG	SER SER	1723	36.152	-7.508	20.160	1.00	46.88
ATOM	2281			1723	35.327	-7.027	21.208	1.00	53.47
ATOM	2284	С	SER	1723	34.088	-8.731	19.359	1.00	46.67
ATOM	2285	O N	SER	1723	32.982	-8.172	19.417	1.00	46.21
ATOM	2283	CA	asn asn	1724	34.237	-10.025	19.590	1.00	47.80
ATOM	2288	CB	ASN ASN	1724	33.092	-10.826	19.999	1.00	52.78
ATOM	2289	CG	asn	1724 1724	32.559 33.679	-10.319	21.355	1.00	57.86
ATOM	2290	OD1	ASN	1724	34.531	-10.091 -10.959	22.370	1.00	61.99
ATOM	2291	ND2	ASN				22.585	1.00	63.17
MOTA	2294	C	asn	1724 1724	33.712 32.015	-8.899 10.770	22.953	1.00	63.56
ATOM	2295	0				-10.779	18.893	1.00	51.43
ATOM	2295	И	ASN CYS	1724	30.859	-10.423	19.108	1.00	51.56
ATOM	2298	CA	CYS	1725	32.454	-11.087	17.683	1.00	48.91
MOTA	2298	CB	CYS	1725 1725	31.600 31.526	-11.136	16.508	1.00	45.62
MOTA	2300	SG	CYS	1725		-9.771 -9.816	15.811	1.00	44.83
ATOM	2300	C	CYS	1725	30.693 32.341	-9.816 -12.135	14.194	1.00	41.83
	2001	_	C13	1/23	24.341	-12.135	15.640	1.00	42.30



ATOM	2367	CA	MET	1732	27.522	-10.777	6.389	1.00	26.47
ATOM	2368	CB	MET	1732	26.562	-11.308	7.458	1.00	25.79
ATOM	2369	CG	MET	1732	25.116	-10.838	7.274	1.00	26.01
ATOM	2370	SD	MET	1732	24.004	-11.550	8.469	1.00	26.22
MOTA	2371	CE	MET	1732	23.787	-13.195	7.783	1.00	23.74
MOTA	2372	C	MET	1732	27.445	~9.243	6.319	1.00	25.15
ATOM	2373	0	MET	1732	26.886	-8.691	5.379	1.00	25.41
MOTA	2374	N	MET	1733	28.024	-8.564	7.308	1.00	26.48
MOTA	2376	CA	MET	1733	28.057	~7.104	7.331	1.00	27.09
MOTA	2377	CB	MET	1733	28.903	-6.594	8.488	1.00	25.91
ATOM	2378	CG	MET	1733	28.235	-6.556	9.824	1.00	31.64
ATOM	2379	SD	MET	1733	29.442	-6.111	11.094	1.00	29.59
ATOM	2380	CE	MET	1733	28.886	-7.126	12.420	1.00	28.14
MOTA	2381	C	MET	1733	28.720	-6.613	6.056	1.00	28.43
MOTA	2382	0	MET	1733	28.185	-5.753	5.372	1.00	31.37
ATOM	2383	N	ARG	1734	29.891	-7.169	5.747	1.00	28.57
ATOM	2385	CA	ARG	1734	30.642	-6.783	4.551	1.00	27.00
ATOM	2386	CB	ARG	1734	32.007	-7.488	4.510	1.00	25.98
ATOM	2387	CG	ARG	1734	32.927	-7.154	5.707	1.00	28.13
ATOM	2388	CD	ARG	1734	33.229	-5.672	5.765	1.00	29.97
ATOM	2389	NE	ARG	1734	33.922	-5.256	4.553	1.00	40.49
ATOM	2391	CZ	ARG	1734	35.238	-5.361	4.363	1.00	43.95
MOTA	2392	NH1	ARG	1734	36.023	-5.853	5.318	1.00	41.81
MOTA	2395	NH2	ARG	1734	35.760	-5.048	3.184	1.00	46.20
ATOM	2398	С	ARG	1734	29.859	-7.037	3.268	1.00	24.57
MOTA	2399	0	ARG	1734	29.992	-6.290	2.314	1.00	24.94
ATOM	2400	N	ASP	1735	29.071	-8.107	3.235	1.00	24.79
ATOM	2402	CA	ASP	1735	28.254	-8.420	2.061	1.00	23.88
MOTA	2403	CB	ASP	1735	27.669	-9.830	2.150	1.00	25.95
MOTA	2404	CG	ASP	1735	28.724	-10.913	2.024	1.00	27.60
ATOM	2405	OD1	ASP	1735	29.842	-10.632	1.529	1.00	27.75
ATOM	2406	OD2	ASP	1735	28.432	-12.051	2.430	1.00	28.90
MOTA	2407	С	ASP	1735	27.139	-7.396	1.941	1.00	22.61
ATOM	2408	0	ASP	1735	26.777	-6.996	0.833	1.00	22.66
ATOM	2409	N	CYS	1736	26.611	-6.965	3.085	1.00	20.61
MOTA	2411	CA	CYS	1736	25.561	-5.952	3.109	1.00	23.63
ATOM	2412	CB	CYS	1736	25.007	-5.767	4.534	1.00	21.98
ATOM	2413	SG	CYS	1736	23.934	-7.126	5.111	1.00	22.95
MOTA	2414	C	CYS	1736	26.129	-4.633	2.599	1.00	23.62
MOTA	2415	0	CYS	1736	25.403	-3.797	2.047	1.00	22.15
MOTA	2416	N	TRP	1737	27.438	-4.461	2.775	1.00	24.37
MOTA	2418	CA	TRP	1737	28.123	-3.247	2.342	1.00	23.77
ATOM	2419	CB	TRP	1737	29.162	-2.810	3.371	1.00	19.38
ATOM	2420	CG	TRP	1737	28.601	-2.520	4.718	1.00	21.62
MOTA	2421	CD2	TRP	1737	29.268	-2.688	5.971	1.00	24.81
ATOM	2422	CE2	TRP	1737	28.371	-2.278	6.980	1.00	25.95
ATOM	2423	CE3	TRP	1737	30.534	-3.165	6.340	1.00	29.02
MOTA	2424	CD1	TRP	1737	27.359	-2.024	5.007	1.00	23.21
MOTA	2425	NE1	TRP	1737	27.213	-1.876	6.362	1.00	21.80
MOTA	2427	CZ2	TRP	1737	28.710	-2.305	8.347	1.00	26.68
MOTA	2428	CZ3	TRP	1737	30.873	-3.198	7.699	1.00	31.06
ATOM	2429	CH2	TRP	1737	29.959	-2.774	8.685	1.00	30.18
ATOM	2430	C	TRP	1737	28.788	-3.372	0.978	1.00	24.88
ATOM	2431	0	TRP	1737	29.737	-2.646	0.689	1.00	25.11
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	ATOM	2432	N	HIS	1720						
	ATOM	2434	CA	HIS	1738	28.3	03 -4	. 278	0.132	1.00	
	ATOM	2435	CB	HIS	1738	28.8	38 -4	.406 -	1.191		25.27
	ATOM	2436	CG		1738	28.2	30 -5		1.986	1.00	24.27
	<b>-</b>	2437	CD2	T	1738	29.17				1.00	25.24
	3	2438			1738	29.72			3.081	1.00	26.28
	_	2440	ND1		1738	29.69		_	4.147	1.00	25.67
				HIS :	1738	30.52			3.098	1.00	27.55
		2441	NE2		1738	30.56			4.117	1.00	27.51
		2443	C	***	1738	28.71		329 -4	1.770	1.00	30.93
		444	0		738	20.71	=	087 - j	. 953	1.00	25.59
		445			739	27.65		451 -1	.905	1.00	
	TOM 2	447	~-			29.784			.612	1.00	22.01
	TOM 2			_	739	29.759			.388		23.84
A			_	_	739	31.131	-1.3		. 024	1.00	24.93
A'		A	_ •		739	28.671	-1.5			1.00	26.39
A.					739	27.963	-0.5		.462	1.00	25.35
				AL 1	740	28.543	_		.727	1.00	28.20
		_		AL 17	740	27.528	-		.073	1.00	22.68
			B V		740	27.995	-2.9		101	1.00	26.46
			G1 V		40	27.995	-3.9				29.70
			'G2 V		40	27.063	-4.0	03 ~8.		_	
AT		57 C				29.433	-3.6			_	26.01
AT		58 O			40	26.213	-3.3		4 4 5		31.22
AT	OM 24		• • •			26.138	-4.47		_		25.07
AT						25.155	-2.51	.9 -5.			23.55
ATO						25.133	-1.19				25.30
ATO						23.844	-2.83			.00 2	2.43
ATC						22.962	-1.67			.00 2	4.09
ATC			PR	0 174	1	23.928					3.12
ATO		_ ~	PR		1	23.272	-0.52			.00 2	2.04
		•	PR	7 174		22.727	-4.19				2.18
ATO			SEI			22.727	-4.90				1.23
ATO			SEI			23.437	-4.57				
ATO		9 CB				22.928	-5.847	7 -7.0			3.87
ATO		O OG	SER		•	23.071	-5.907	-8.6			. 36
ATO		2 C	SER		_	24.436	-6.025				7.39
ATON	4 2473					23.636	-7.058				25
ATON		_	SER			3.145	-8.179				. 96
ATOM			GLN	_		4.810	-6.839			00 24	.30
ATOM			GLN		2	5.558	-7.934			00 24	. 39
ATOM	,,		GLN	1743	2	7.046		-5.34			.15
ATOM			GLN	1743	2	7.359	-7.755	~5.63		00 23	. 83
ATOM			GLN	1743	2	6.816	-7.784	-7.12	6 1.0		. 84
ATOM	•	OE1	GLN	1743			-9.036	-7.80	8 1.0		
	~	NE2	GLN	1743	21	7.318 5.775	10.135	-7.59	0 1.0		
ATOM	2484	C	GLN	1743	2.	- 222	-8.871	-8.62	8 1.0		
ATOM	2485	Ö	GLN	1743	2:	5.309	-8.171	-3.86	3 1.0		45
ATOM	2486	N	ARG		25	816	-9.135	-3.31	7 1.0		
ATOM	2488	CA		1744	24	.557	-7.280	-3.225		•	
ATOM	2489	СВ	ARG	1744	24	.242	-7.424			•	
ATOM	2490		ARG	1744	23		-6.110	-1.806			11
ATOM		CG	ARG	1744	24		-4.959	-1.231		0 19.	70
ATOM	2491	CD	ARG	1744	24			-1.338		21.	
ATOM	2492	NE	ARG	1744	24		-3.640	-0.890		20.	
	2494	CZ	ARG	1744		_	2.552	-1.305	1.00		
ATOM	2495	NH1	ARG	1744			1.313	-1.583	1.00		
ATOM	2498	NH2	ARG	1744			0.955	-1.481	1.00		
MOTA	2501	C	ARG		25.	450 -	0.448	-2.036	1.00		
		-	AUG.	1744	23.		8.505	-1.640			
SSSD/55	145. v01						-	040	1.00	22.5	3
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MOTA	2502	0	ARG	1744	22.437	-8.800	-2.588	1.00	23.08
ATOM	2503	N	PRO	1745	23.162	-9.170	-0.467	1.00	20.76
MOTA	2504	CD	PRO	1745	24.087	-9.078	0.681	1.00	21.71
ATOM	2505	CA	PRO	1745	22.160	-10.207	~0.243	1.00	22.34
ATOM	2506	CB	PRO	1745	22.632	-10.859	1.057	1.00	20.58
MOTA	2507	CG	PRO	1745	23.298	-9.727	1.783	1.00	20.36
MOTA	2508	C	PRO	1745	20.814	-9.512	-0.048	1.00	23.62
MOTA	2509	0	PRO	1745	20.759	-8.318	0.255	1.00	25.29
ATOM	2510	N	THR	1746	19.731	-10.235	-0.275	1.00	23.39
ATOM	2512	CA	THR	1746	18.404	-9.675	-0.080	1.00	22. <b>7</b> 7
ATOM	2513	CB	THR	1746	17.386	-10.368	-1.004	1.00	23.24
MOTA	2514	OG1	THR	1746	17.409	-11.783	-0.763	1.00	23.11
ATOM	2516	CG2	THR	1746	17.724	-10.103	-2.475	1.00	24.96
ATOM	2517	С	THR	1746	18.009	-9.954	1.365	1.00	24.98
ATOM	2518	0	THR	1746	18.664	-10.758	2.043	1.00	24.30
MOTA	2519	N	PHE	1747	16.944	-9.318	1.853	1.00	24.95
ATOM	2521	CA	PHE	1747	16.501	-9. <b>59</b> 6	3.221	1.00	25.16
ATOM	2522	CB	PHE	1747	15.395	-8.628	3.661	1.00	23.64
MOTA	2523	CG	PHE	1747	15.916	-7.283	4.089	1.00	24.34
ATOM	2524	CD1	PHE	1747	16.715	-7.167	5.226	1.00	21.21
ATOM	2525	CD2	PHE	1747	15.649	-6.137	3.334	1.00	21.42
ATOM	2526	CE1	PHE	1747	17.252	-5.932	5.597	1.00	20.99
ATOM	2527	CE2	PHE	1747	16.178	-4.907	3.699	1.00	20.36
MOTA	2528	CZ	PHE	1747	16.985	-4.807	4.840	1.00	19.30
ATOM	2529	С	PHE	1747	16.034	-11.049	3.311	1.00	23.57
ATOM	2530	0	PHE	1747	16.182	-11.702	4.344	1.00	25.32
ATOM	2531	N	LYS	1748	15.520	-11.573	2.202	1.00	23.19
ATOM	2533	CA	LYS	1748	15.066	-12.958	2.167	1.00	23.67
ATOM	2534	CB	LYS	1748	14.462	-13.285	0.799	1.00	26.67
MOTA MOTA	2535	CG	LYS	1748	14.018	-14.739	0.622	1.00	30.49
ATOM	2536	CD	LYS	1748	13.642	-14.996	-0.837	1.00	38.98
	2537	CE	LYS	1748	13.182	-16.432	-1.087	1.00	44.52
ATOM ATOM	2538 2542	NZ	LYS	1748	11.997	-16.790	-0.245	1.00	52.75
ATOM	2542 2543	С О	LYS	1748	16.264	-13.865	2.445	1.00	25.65
ATOM	2544	N	LYS GLN	1748	16.184	-14.778	3.270	1.00	27.19
MOTA	2544	CA	GLN	1749	17.378	-13.603	1.762	1.00	24.56
ATOM	2547	CB	GLN	1749 1749	18.588	-14.397	1.950	1.00	26.33
ATOM	2548	CG	GLN	1749	19.702 19.416	-13.953 -14.066	0.993 -0.484	1.00	27.97
ATOM	2549	CD	GLN	1749	20.518	-13.415	-1.315	1.00	37.31
ATOM	2550	OE1	GLN	1749	20.318			1.00	40.24
ATOM	2551	NE2	GLN	1749	21.726	-12.408 -13.983	-1.970	1.00	38.83
ATOM	2554	C	GLN	1749	19.099	-14.223	-1.259 3.377	1.00	47.83
ATOM	2555	o	GLN	1749	19.459	-15.196		1.00	23.92
ATOM	2556	N	LEU	1750	19.155	-12.976	4.040	1.00	25.27
ATOM	2558	CA	LEU	1750	19.641	-12.662	3.829	1.00	23.12
ATOM	2559	CB	LEU	1750	19.607	-11.149	5.175 5.427	1.00	24.34
ATOM	2560	CG	LEU	1750	20.633	-10.311		1.00	23.08
ATOM	2561	CD1	LEU	1750	20.833	-8.806	4.665 4.724	1.00	23.84
ATOM	2562	CD2	LEU	1750	22.013	-10.586	5.246	1.00	22.10
ATOM	2563	C	LEU	1750	18.840	-13.400			24.91
ATOM	2564	0	LEU	1750	19.408	-13.400	6.236	1.00	27.40
ATOM	2565	N	VAL	1751	17.527	-13.482	7.211 6.031	1.00 1.00	27.11
ATOM	2567	CA	VAL	1751	16.665	-13.462	6.970	1.00	26.83
	'				20.000	44.4/4	0.5/0	1.00	25.31

							7	.56				
A:	rom 2	568	CB (	/AL 1	751							
A	rom 2				751	15.1		-13.9		599	1.0	00 25.87
AT	TOM 2!				751	14.3		-14.9		382	1.0	
		571. (	_		751	14.7 17.0		-12.5	93 6.	934	1.0	0 21.52
		572 C			751	17.1		-15.6		025	1.0	0 25.87
		73 N			752	17.2		-16.2		106	1.0	
					52	17.6		-16.2		858	1.0	0 29.98
AT	. –				52	17.6		-17.6		799	1.0	
AT		77 C	G G		52	16.28		-18.1; -18.0;		346	1.0	
ATO		_	D G	LU 17	52	16.30		-18.57		570	1.0	
ATO			El GI			15.45		-18.12	•		1.00	· · ·
AT(			E2 GI	Մ 17	52	17.15		-19.42			1.00	
ATC ATC			GI	U 17	52	18.99		-17.89	_		1.00	
ATC			GI	U 17	52	19.17		-18.84			1.00	
ATC			AS		53	19.95		-17.01			1.00	
ATO					53	21.27		-17.13			1.00	
ATO				_	3	22.24		-16.10			1.00	
ATO					-	22.48		-16.34			1.00	
ATO					3	22.36		-17.49			1.00	
ATO						22.819		-15.37			1.00	
ATO		_	AS			21.215	ò	-16.968			1.00	38.26
ATON		_	ASI			21.739	)	-17.800			1.00	28.54
ATON			LE			20.537	'	-15.926			1.00	28.95
ATOM			LEU			20.421		-15.673			1.00	27.25
ATOM			LEU LEU	_		19.754		-14.328	10.45	_	1.00	28.08 23.31
ATOM						20.733		13.199	10.16		1.00	24.47
ATOM	2598					20.007		11.863	10.09		1.00	19.58
ATOM	2599		LEU			21.846		13.207	11.21		1.00	21.17
ATOM	2600	0	LEU			19.688		16.789	10.92		1.00	31.61
MOTA	2601	N	ASP	1755		20.037		17.135	12.04	3	1.00	32.64
MOTA			ASP	1755		18.690 17.931		17.367	10.25		1.00	32.61
ATOM	2604	CB	ASP	1755		16.823		18.460	10.833		1.00	34.20
ATOM	2605	CG	ASP	1755		15.808		18.883	9.872	_	L.00	37. <b>7</b> 0
ATOM	2606	OD1	ASP	1755		15.445		19.780	10.526		00	44.27
ATOM	2607	OD2	ASP	1755		15.370		19.521	11.692		.00	47.16
ATOM	2608	С	ASP	1755		18.894		20.745 19.616	9.876		.00	51.35
ATOM	2609	0	ASP	1755		18.858		20.273	11.073		.00	34.63
ATOM ATOM	2610	N	ARG	1756		19.782		19.826	12.119	_	.00	36.24
ATOM	2612	CA	ARG	1756	:	20.784		20.870	10.108 10.190		.00	32.60
ATOM	2613	CB	ARG	1756		21.548		0.939	8.867		.00	33.69
ATOM	2614	CG	ARG	1756	2	22.639		2.003	8.800		.00	35.42
ATOM	2615 2616	CD	ARG	1756		23.212		2.094	7.395		.00	40.87
ATOM	2618	NE	ARG	1756	2	23.739		0.813	6.926			42.73
ATOM	2619	CZ	ARG	1756	2	4.882	-2	0.274	7.340			48.45
ATOM	2622.	NH1	ARG	1756		5.634		0.905	8.243			49.90
ATOM	2625	NH2	ARG	1756	2	5.276	-1	9.105	6.844			49.63
ATOM	2626	C O	ARG	1756		1.748	- 2	0.598	11.345			50.86
ATOM	2627	Ŋ	ARG	1756		1.929	-2	1.436	12.228			34.78
ATOM	2629	CA	ILE	1757		2.325	-1	9.402	11.363			36.24
ATOM	2630	CB	ILE	1757		3.281	-19	9.018	12.392			35.35 35.54
ATOM	2631	CG2	ILE	1757		3.905	-17	7.631	12.103	1.		34.99
ATOM	2632	CG1	ILE	1757		4.955	~17	7.303	13.159	1.	_	32.06
•	- <del>-</del>		- 11E	1757	24	4.547	-17	7.626	10.711	1.		13.77
SSSD/FF										-		





					15	•			
						26 247	10.185	1.00	31.44
n moM	2633	CD1	ILE	1757	24.908	-16.247	13.803	1.00	36.49
MOTA	2634	C	ILE	1757	22.698	-19.036	14.716	1.00	36.40
MOTA	2635	0	ILE	1757	23.337	-19.548	13.988	1.00	36.91
MOTA	2636	N	VAL	1758	21.487	-18.515	15.322	1.00	38.68
MOTA		CA	VAL	1758	20.881	-18.498	15.312	1.00	37.77
MOTA	2638	CB	VAL	1758	19.425	-17.962		1.00	38.39
MOTA	2639	CG1	VAL	1758	18.806	-18.059	16.708	1.00	36.69
MOTA	2640	CG2	VAL	1758	19.392	-16.524	14.854	1.00	41.38
MOTA	2641		VAL	1758	20.891	-19.908	15.895	1.00	42.41
MOTA	2642	C	VAL	1758	21.405	-20.138	16.997	1.00	
MOTA	2643	0	ALA	1759	20.379	-20.851	15.111	1.00	
MOTA	2644	N	ALA	1759	20.325	-22.247	15.508	1.00	
MOTA	2646	CA		1759	19.741	-23.074	14.384		
MOTA	2647	CB	ALA	1759	21.703	-22.787	15.897	1.00	
ATOM	2648	C	ALA	1759	21.822	-23.594	16.809	1.00	
MOTA	2649	0	ALA	1760	22.740	-22.339	15.208	1.00	
MOTA	2650	N	LEU	1760	24.095	-22.800	15.493	1.00	
MOTA	2652	CA	LEU	1760	24.921	-22.761	14.203	1.00	
MOTA	2653	CB	LEU	1760	24.286	-23.545	13.060		
MOTA	2654	CG	LEU		24.973	-23.222	11.745		
MOTA	2655				24.343	-25.038	13.369		
MOTA	2656	CD2			24.811	-21.986	16.573		
MOTA		C	LEU		25.917		16.989		
ATOM		3 0	LEU		24.183		17.034		
ATOM		) N	THE		24.814		18.02		
ATOM		L CA	THE		24.314		17.83	1.0	
ATON		2 CB	THE		24.382		7 16.52	9 1.0	
ATON		3 OG:			25.063			3 1.0	0 48.64
MOTA		5 CG			24.673	_			
ATO		6 C	TH			_		7 1.0	
ATO		_	TH		23.584		_	6 1.0	
ATO	~ ~ ~	8 N	SE		25.81				00 50.98
OTA			SE					2 1.0	
ATO		_	SE					8 1.0	00 57.99
ATO		_	; SE						00 49.39
ATC			SE	R 1762					00 48.00
ATC		_	SE	R 1762	25.29				00 48.84
ATC			SE		79.62				00 46.93
TA			A SI		79.56		_	09 1.	00 46.66
ATO			B SI	ER 461	78.27				00 43.02
ATC			S	ER 461	79.67			10 1.	00 40.19
AT		79 0	S	ER 461	79.69				.00 41.48
TA		80 N	G	LU 462	79.79		_		.00 39.59
			A G	LU 462	79.9				.00 40.66
				LU 462	80.03				.00 36.60
		84 0		LU 462	81.0				.00 35.10
		185	_	LU 462	80.8		· <del>-</del> -		.00 36.07
	_			YR 463	82.2		. – .		.00 35.60
		-		YR 463	83.4			-	.00 38.15
				YR 46	84.5				.00 44.08
				ryr 46	3 84.3				00 44.99
				TYR 46	3 84.1		-		.00 46.88
	_			TYR 46		333 30.			L.00 43.95
				TYR 46		305 27.			1.00 41.86
				TYR 46			044 6.	642	L. 00
A	TOM 3	494	CEZ						



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	ATOM	3495	CZ	TYR	463		_					
4	ATOM	3496	ОН	TYR		,			282	7.215	1.00	12.5-
		3498	С	TYR	463		68	31.	364	6.431		
	MOTA	3499	0		463	93.7	03	24.		10.014		,
7		3500	N	TYR	463	84.4	40	23.			_	-5.50
		3502		GLU	464	83,7	42	24.0		9.147		•
			CA	GLU	464	84.1		22.7		1.260	1.00	32.81
		3503	CB	GLU	464	85.66				1.633	1.00	34.64
		504	CG	GLU	464	86.07	7-	22.7		1.919	1.00	37.48
		505	CD	GLU	464			23.6		3.049	1.00	45.48
	TOM 3	506		GLU	464	87.55		23.9		3.015	1.00	
				GLU		87.92	0	24.9		3.659		55.80
A:	TOM 3	~	_		464	88.34	4	23.2		2.351	1.00	61.78
A?			_	GLU	464	83.42	6	22.2			1.00	58.34
		• • •	. •	3LU	464	83.08		23.1		2.858	1.00	33.05
				EU	465	83.14		21 04		3.705	1.00	34.54
				ĿΕÜ	465	82.462		21.00		.943	1.00	32.59
			B I	EU	465			20.46		.114	1.00	33.74
	OM 35	14 c	G I	EU	465	81.484	4	19.34		.747	1.00	
AT		15 C				80.510		19.43		.577	1.00	31.20
AT	OM 35		-		465	79.355	5	18.49	_	.858		32.77
AT		_	_		465	80.021		20.84		.359	1.00	26.22
ATO			_		465	83.511		19.88			1.00	31.59
ATO					465	84.641		19.57		.059	1.00	35.64
ATO	- •			२० ४	166	83.150				642	1.00	33.77
ATO	_		D PI	₹0 4	166	81.865		19.73		349	1.00	36.71
				0 4	166	84.074		20.104		967	1.00	36.97
ATO		22 CE	PF	_	66	03.0/4		19.185			_	36.17
ATO		3 CG			66	83.247		19.196	18.			
ATO		4 C	PR	_ ~		82.274	:	20.326	18.			36.83
ATO	M 352			_	66	84.419		17.765		<b>-</b>		40.80
ATO		•	PR	_	66	83.626		L7.077			1.00	37.39
ATO		_	GL	_	67	85.611		7.330				34.71
ATO		_	GL	_	67	86.030		.5.987			1.00	8.40
ATON			GL	J 40	57	87.493			16.9			2.59
ATOM		•••	GL	J 46	57	87.922		5.987	16.5			9.21
			GL	J 46	57	89.276		4.682	15.8			8.93
ATOM	-054		GLt			90.276		4.769	15.2	13 1		4.76
ATOM		OE2				90.013		5.767	15.4		_	
ATOM		C	GLU			89.592	1.	3.823	14.4			3.57
ATOM	3535		GLU			85.825		5.037	18.1			9.03
ATOM	3536	_				85.938	15	5.430	19.3			0.74
ATOM	3538		ASP			85.472	13	3.802				l.52
ATOM	3539		ASP	46		85.273		2.776	17.8		.00 38	3.57
ATOM		CB	ASP	46	8	83.793		.640	18.8		.00 40	.86
ATOM	3540	CG	ASP	468	3	83.566			19.22	24 1.		.27
	3541	OD1	ASP	468	3	82.429		.697	20.39	97 1.		. 36
ATOM	3542	OD2	ASP	468		04 514		.670	20.91			. 50
MOTA	3543	C	ASP	468		84.514		.992	20.80	7 1.		.55
ATOM	3544	0	ASP			85.803	11	.470	18.27			
ATOM	3545	N		468		85.068	10	. 701	17.65		_	. 75
ATOM	3546		PRO	469	•	87.100		.209				. 80
ATOM	3547	CD	PRO	469	٤	38.001		. 062	18.48			. 71
ATOM		CA	PRO	469	8	37.801			19.27		00 41	
	3548	CB	PRO	469	<u>-</u> ۾	9.091	10.	011	18.01		00 40.	
ATOM	3549	CG	PRO	469	_		10.	042	18.83		0 40.	
MOTA	3550	С	PRO	469		9.366	11.	505	18.938	3 1.0		
MOTA	3551	0	PRO			7.033	8.		18.260			
ATOM	3552	N		469	8	7.032			17.414			
ATOM	3554		ARG	470	8	6.361			19.411		•	
-		CA	ARG	470	8	5.600						70
SSSD/55	145 ^-					-	•		19.779	1.0	0 41.	03





ATOM	3555	CB	ARG	470	84.827	7.677	21.075	1.00	44.18
ATOM	3556	CG	ARG	470	85.628	8.240	22.218	1.00	47.89
ATOM	3557	CD	ARG	470	84.719	8.518	23.400	1.00	50.56
ATOM	3558	NE	ARG	470	83.576	9.345	23.023	1.00	51.20
ATOM	3560	CZ	ARG	470	82.6 <b>9</b> 5	9.845	23.881	1.00	52.24
ATOM	3561	NH1	ARG	470	82.818	9.608	25.183	1.00	51.31
ATOM	3564	NH2	ARG	470	81.672	10.564	23.432	1.00	52.73
ATOM	3567	С	ARG	470	84.596	7.004	18.723	1.00	39.03
MOTA		0	ARG	470	84.401	5.813	18.518	1.00	40.72
ATOM	3569	N	TRP	471	83.972	7.965	18.050	1.00	37.77
ATOM	3571	CA	TRP	471	82.948	7.656	17.059	1.00	36.73
ATOM	3572	СВ	TRP	471	81.672	8.401	17.432	1.00	35.05
ATOM	3573	CG	TRP	471	81.044	7.862	18.673	1.00	34.85
ATOM	3574	CD2	TRP	471	80.235	6.687	18.766	1.00	34.96
ATOM	3575	CE2	TRP	471	79.831	6.564	20.116	1.00	35.12
MOTA	3576	CE3	TRP	471	79.810	5.721	17.838	1.00	33.25
ATOM		CD1	TRP	471	81.106	8.390	19.933	1.00	29.97
ATOM	3578	NE1	TRP	471	80.377	7.616	20.805	1.00	32.18
ATOM	3580	CZ2	TRP	471	79.017	5.512	20.560	1.00	33.98
ATOM	3581	CZ3	TRP	471	79.002	4.673	18.282	1.00	33.71
ATOM	3582	CH2	TRP	471	78.618	4.580	19.632	1.00	33.28
ATOM	3583	С	TRP	471	83.275	7.930	15.599	1.00	37.27
ATOM	3584	0	TRP	471	82.580	7.445	14.695	1.00	36.61
ATOM	3585	N	GLU	472	84.341	8.680	15.361	1.00	37.93
ATOM	3587	CA	GLU	472	84.706	9.054	14.004	1.00	37.08
ATOM	3588	СВ	GLU	472	85.865	10.049	14.045	1.00	36.30
MOTA	3589	CG	GLU	472	86.026	10.851	12.773	1.00	33.51
ATOM	3590	CD	GLU	472	84.931	11.895	12.580	1.00	33.80
ATOM	3591	OE1	GLU	472	84.385	12.408	13.581	1.00	35.19
MOTA	3592	OE2	GLU	472	84.641	12.226	11.412	1.00	32.51
ATOM	3593	С	GLU	472	85.021	7.923	13.032	1.00	37.88
ATOM	3594	0	GLU	472	85.774	7.000	13.351	1.00	38.20
ATOM	3595	N	LEU	473	84.422	7.992	11.846	1.00	37.55
ATOM	3597	CA	LEU	473	84.678	7.004	10.813	1.00	36.93
ATOM	3598	CB	LEU	473	83.404	6.244	10.443	1.00	37.08
MOTA	3599	CG	LEU	473	83.680	5.086	9.470	1.00	39.14
MOTA	3600	CD1	LEU	473	84.196	3.877	10.250	1.00	38.39
MOTA	3601	CD2	LEU	473	82.433	4.716	8.672	1.00	39.46
MOTA	3602	С	LEU	473	85.207	7.732	9.577	1.00	38.52
MOTA	3603	0	LEU	473	84.660	8.764	9.182	1.00	38.67
ATOM	3604	N	PRO	474	86.334	7.259	9.005	1.00	39.02
MOTA	3605	CD	PRO	474	87.259	6.259	9.571	1.00	38.39
ATOM	3606	CA	PRO	474	86.918	7.877	7.809	1.00	38.24
ATOM	3607	CB	PRO	474	88.188	7.049	7.590	1.00	38.40
MOTA	3608	CG	PRO	474	88.580	6.680	8.979	1.00	35.50
ATOM	3609	C	PRO	474	85.942	7.727	6.642	1.00	37.56
MOTA	3610	0	PRO	474	85.415	6.641	6.400	1.00	37.88
MOTA	3611	N	ARG	475	85.720	8.809	5.907	1.00	37.73
ATOM	3613	CA	ARG	475	84.779	8.790	4.795	1.00	40.01
MOTA	3614	CB	ARG	475	84.655	10.183	4.182	1.00	38.31
MOTA	3615	CG	ARG	475	84.217	11.236	5.198	1.00	35.15
MOTA	3616	CD	ARG	475	84.069	12.631		1.00	33.92
ATOM	3617	NE	ARG	475	83.718	13.603	5.616	1.00	30.45
MOTA	3619	CZ	ARG	475	82.475	13.880	5.993	1.00	26.48
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		3620	NH1	ARG	475	01 44						
		3623	NH2		475	81.44 82.27		284	5.4		.00	24.80
		626	_		475	85.05		650	7.0		.00	25.16
		627	0		475	84.12	· · · · · · · · · · · · · · · · · · ·	735	3.7		.00	42.18
		628			176	86.32		197	3.1			41.43
				ASP 4	76	86.67	-	391 387	3.5		.00	45.44
				ASP 4	76	88.19		30/ 343	2.5		00	49.80
				ASP 4	76	88.944	_	975	2.32			50.95
		'			76	89.303		789	3.58			3.89
			_		76	89.176		367	3.73			9.71
					76	86.149			4.42	_		7.39
AT			_		76	86.051			2.95 2.12		_	1.23
AT					77	85.814	4.8		4.23			3.54
ATO					77	85.285	3.6		4.75			0.49
ATO		_			77	85.834	3.3		6.15			9.32
ATO		_			77	87.237	2.8		6.112			9.79
ATO		_	_	RG 47		87.960	2.9		7.420			3.06
ATO						87.310	2.2		8.529			5.76
ATC						87.728	2.3		9.789			3.35
ATO						88.793	3.10		10.101			2.23
ATO			AR			87.067	1.74		10.745		_	.66
ATO	M 365		AR	•		83.755	3.54	7	4.750			.35 .04
ATO	M 365	4 N	LE			83.160	2.69		5.404			.09
ATO	M 365	6 CA				83.129	4.41		3.958	1.00		.38
ATO		7 CB				81.685	4.46		3.870	1.00		.60
ATO						81.168	5.57		4.790	1.00		. 39
ATON		9 CD				79.651	5.69		4.894	1.00		. 38
ATOM		O CD	2 LE			79.113 79.293	4.59		5.802	1.00		
ATOM		_	LEU			81.279	7.06		5.441	1.00	40.	
ATOM		_	LEU	478		81.696	4.774	_	2.433	1.00	41.	
ATOM ATOM			VAL	479		80.466	5.780 3.904		1.870	1.00	43.	
ATOM			VAL	479		79.992	4.082		1.844	1.00	42.	29
ATOM			VAL			80.227	2.816		0.471	1.00	41.	
ATOM	3667 3668	_				79.719	3.057		0.397	1.00	41.	
ATOM	3669		_	479		81.700	2.448		1.810 0.420	1.00	40.	
ATOM	3670	•	VAL	479		78.500	4.345		0.420	1.00	41.	
ATOM	3671	N O	VAL	479		77.719	3.451		).885	1.00	40.4	
ATOM	3673	CA	LEU	480		78.112	5.582		253	1.00	39.8	
ATOM	3674	CB	LEU	480		76.706	5.973		.293	1.00	41.3	
ATOM	3675	CG	LEU	480		76.568	7.492		.166	1.00	41.6	
ATOM	3676	CD1	LEU	480		77.236	8.332		.261	1.00	39.9	
ATOM	3677	CD2	LEU	480		76.890	9.800		.039	1.00	39.2 37.7	
ATOM	3678	C	LEU	480 480		76.791	7.877		.647	1.00	35.1	
ATOM	3679	0	LEU	480		75.899	5.273			1.00	42.2	
ATOM	3680	N	GLY	481		76.395	5.048			1.00	45.2	
ATOM	3682	CA	GLY	481		74.650	4.947			1.00	41.5	
ATOM	3683	C	GLY	481		73.812	4.257	-1.	433	1.00	40.19	
ATOM	3684	0	GLY	481		2.446	4.872	-1.	640	1.00	41.58	
ATOM	3685	N	LYS	482		2.262	6.091		550	1.00	41.35	
ATOM	3687	CA	LYS	482		1.474	4.009		908	1.00	42.65	
ATOM	3688	CB	LYS	482		0.105 9.240	4.429		166 1	1.00	44.17	
ATOM	3689	С	LYS	482		9.475	3.221		542 1	1.00	45.66	
\$\$\$D/5.5	1.45				J	3 ( )	5.148	-0.	994 1	.00	44.86	

ATOM	3690	0	LYS	482	69.638	4.752	0.155	1.00	45.23
ATOM	3691	N	PRO	483	68.749	6.234	-1.273	1.00	45.94
MOTA	3692	CD	PRO	483	68.518	6.880	-2.576	1.00	46.96
ATOM	3693	CA	PRO	483	68.099	6.983	-0.206	1.00	47.79
MOTA	3694	CB	PRO	483	67.542	8.200	-0.947	1.00	47.02
MOTA	3695	CG	PRO	483	67.269	7.666	-2.307	1.00	46,65
ATOM	3696	C	PRO	483	66.991	6.151	0.429	1.00	48.74
ATOM	3697	0	PRO	483	66.314	5.376	-0.251	1.00	48.01
ATOM	3698	N	LEU	484	66.858	6.268	1.742	1.00	49.91
ATOM	3700	CA	LEU	484	65.837	5.547	2.477	1.00	53.93
MOTA	3701	CB	LEU	484	66.433	4.883	3.720	1.00	50.17
MOTA	3702	CG	LEU	484	67.517	3.844	3.445	1.00	48.93
ATOM	3703	CD1	LEU	484	68.226	3.460	4.731	1.00	49.05
ATOM	3704	CD2	LEU	484	66.906	2.630	2.784	1.00	47.03
ATOM	3705	C	LEU	484	64.715	6.501	2.878	1.00	58.70
ATOM	3706	0	LEU	484	63.571	6.075	3.055	1.00	61.95
ATOM	3707	N	GLY	485	65.027	7.788	3.006	1.00	60.35
ATOM	3709	CA	GLY	485	63.998	8.737	3.397	1.00	64.00
MOTA	3710	C	GLY	485	64.445	10.183	3.476	1.00	66.09
MOTA MOTA	3711	0	GLY	485	65.643	10.468	3.577	1.00	65.26
ATOM	3712 3714	N CA	GLU	486	63.471	11.090	3.458	1.00	67.18
ATOM	3715	CB	GLU GLU	486	63.733	12.525	3.508	1.00	68.69
ATOM	3716	СВ	GLU	486 486	63.873	13.084	2.091	1.00	69.88
ATOM	3717	0	GLU	486	62.618	13.249	4.245	1.00	68.80
ATOM	3718	N	GLY	487	61.481	12.775	4.295	1.00	69.26
ATOM	3720	CA	GLY	487	62.943 61.960	14.415 15.188	4.791	1.00	68.47
ATOM	3721	C	GLY	487	62.373	16.635	5.520 5.634	1.00	67.56
ATOM	3722	Ö	GLY	487	63.040	17.172	4.747	1.00	66.71
ATOM	3723	N	ALA	488	61.979	17.172	6.735	1.00	66.48 67.22
ATOM	3725	CA	ALA	488	62.304	18.661	6.992	1.00	67.78
ATOM	3726	CB	ALA	488	61.637	19.121	8.283	1.00	68.97
MOTA	3727	С	ALA	488	63.817	18.830	7.085	1.00	67.38
MOTA	3728	0	ALA	488	64.413	18.597	8.141	1.00	67.14
MOTA	3729	N	PHE	489	64.429	19.155	5.946	1.00	66.22
ATOM	3731	CA	PHE	489	65.877	19.364	5.831	1.00	65.49
MOTA	3732	CB	PHE	489	66.277	20.699	6.467	1.00	66.11
ATOM	3733	С	PHE	489	66.749	18.207	6.368	1.00	64.07
ATOM	3734	0	PHE	489	67.924	18.399	6.731	1.00	61.56
MOTA	3735	N	GLY	490	66.171	17.005	6.349	1.00	60.79
MOTA	3737	CA	GLY	490	66.852	15.803	6.797	1.00	54.72
ATOM	3738	С	GLY	490	66.787	14.760	5.692	1.00	51.78
ATOM	3739	0	GLY	490	65.765	14.624	5.013	1.00	49.17
ATOM	3740	N	GLN	491	67.874	14.015	5.528	1.00	49.97
ATOM	3742	CA	GLN	491	68.000	12.984	4.504	1.00	48.06
ATOM	3743	CB	GLN	491	68.891	13.520	3.371	1.00	51.02
ATOM	3744	CG	GLN	491	69.286	12.518	2.289	1.00	56.00
MOTA	3745	CD	GLN	491	70.155	13.143	1.202	1.00	58.93
ATOM	3746	OE1	GLN	491	70.483	14.330	1.255	1.00	60.31
ATOM	3747	NE2	GLN	491	70.529	12.341	0.202	1.00	60.19
ATOM	3750	C	GLN	491	68.623	11.720	5.114	1.00	45.59
MOTA	3751	0	GLN	491	69.511	11.792	5.959	1.00	45.22
MOTA	3752	N	VAL	492	68.148	10.561	4.693	1.00	43.19
ATOM	3754	CA	VAL	492	68.676	9.304	5.193	1.00	41.54

_							102					
	ATOM	3755	CB	VAL	492	67 6						
		3756	CG1	VAL	492	•		8.584	6.0	87 1	.00	41.74
		3757	CG2	VAL	492			7.248	6.5		.00	43.70
A	ATOM 3	3758	C	VAL	492			9.463	7.2		.00	
A	ATOM 3	3759	0	VAL		68.9	71	8.424	3.9		.00	44.07
A	TOM 3	760	N	VAL	492	68.1	25 չ	3.271	3.10		.00	39.72
A		762			493	70.1	76	7.872	3.94			39.81
		763		VAL	493	70.54		7.001	2.84		.00	36.38
				VAL	493	71.58		.666			00	35.88
				VAL	493	71.14		.069	1.86	_	00	36.92
	_			VAL	493	72.97		.670	1.48		00	36.64
				VAL	493	71.13			2.46		00	38.29
			0 1	VAL	493	71.69		.689	3.35		00	36.03
			N j	LEU	494	70.94	_	.617	4.44		00	36.57
		770 (	CA I	LEU	494	70.94		.637	2.57	1 1.6		34.91
		71 (		EU	494	71.50		.344	2.90	9 1.(		36.04
AT	'OM 37	72 (		_	494	70.80		. 244	2.094			
AT	OM 37	_	-			71.312		814	2.269			37.43
AT				_	494	71.327	70.	437	3.735			36.62
ATO		_	_		494	70.419		118				36.37
ATO		~			494	72.967		451	1.479			10.70
ATO					494	73.308		160	2.510			37.08
ATO	- ,	<b>-</b> -	• • •	LA 4	495	73.839	· ·		1.560	_	0 3	4.90
ATC			A A	LA 4	195	75.246		779	3.243	1.0		7.18
			B Al	LA 4	195	75.885		830	2.918	1.0		9.84
ATO			AI	LA 4	95	75.949		066	3.541	1.00		9.29
ATO		2 0	AI	_	95			578	3.400	1.00		1.68
ATO	_	3 N	GI	_	96	75.400		808	4.189	1.00		1.53
ATO		5 CA		_	96	77.149	1.3	348	2.881	1.00	_	3.44
ATO	M 378	6 CE		_		77.936	0.2		3.297	1.00		
ATO				_	96	78.328	-0.6	63	2.101	1.00		2.86
ATOM	M 378				96	77.120	-1.1		1.320			1.63
ATO					96	77.386	-2.4		0.545	1.00		3.31
ATOM				•	96	76.494	-3.3			1.00		.48
ATOM						78.477	-2.5		0.534	1.00		.39
ATOM			GL	J 49	96	79.150	0.7		0.053	1.00	62	.15
ATOM			GL		96	79.889	1.5		4.006	1.00	40	. 96
ATOM			ALA	49	7	79.267			3.455	1.00	40	.81
	4.55		ALA	49	7	80.381	0.43		5.280	1.00	40	.79
ATOM			ALA	49	7	79.888	0.85	_	5.096	1.00		. 84
ATOM	,	_	ALA				1.24		7.478	1.00		. 80
ATOM	3798	0	ALA			81.394	-0.28		.181	1.00	44.	
ATOM	3799	N	ILE			81.019	-1.44	5 6	.215	1.00	44.	
ATOM	3801	CA	ILE			82.678	0.05	4 6	.183	1.00		
ATOM	3802	СВ	ILE			83.729	-0.95	2 6	.255	1.00	48.	
ATOM	3803	CG2		498		84.654	-0.89				48.	
ATOM	3804		ILE	498		85.748	-1.95			1.00	50.	
ATOM	3805	CG1	ILE	498		83.851	-1.10			1.00	51.	
ATOM	3806	CD1	ILE	498	3	83.139	0.146			1.00	51.	
ATOM		С	ILE	498	t ,	84.573	-0.754			1.00	55.	47
	3807	0	ILE	498		85.005			. 511	1.00	48.	31
ATOM	3808	N	GLY	499		34.754	0.359		805	1.00	47.	
ATOM	3810	CA	GLY	499			-1.829		271	1.00	49.	
ATOM	3811	C	GLY	499		35.563	-1.774		479	1.00	53.1	
ATOM	3812	0	GLY	499	-	35.076	-0.944	10.		00	57.2	
ATOM	3813	N	LEU	500		5.885	-0.341	11.				
ATOM	3815	CA			8	3.768	-0.948				59.2	
ATOM	3816	CB	LEU	500		3.193	-0.189				58.5	
		CB	LEU	500	8	1.705	-0.519	12.			57.8	
SSSD/sc								+2.	727 J	.00	55.6	7

MOTA	3817	CG	LEU	500	80.789	0.036	11.086	1.00	54.81
ATOM	3818	CD1	LEU	500	79.361	-0.445	11.293	1.00	53.00
MOTA	3819	CD2	LEU	500	80.854	1.561	11.089	1.00	53.27
MOTA	3820	С	LEU	500	83.926	-0.466	13.333	1.00	58.15
MOTA	3821	0	LEU	500	84.461	-1.560	13.529	1.00	60.29
MOTA	3822	N	PRO	505	87.397	-6.022	10.511	1.00	77.18
ATOM	3823	CD	PRO	505	88.509	-6.651	11.242	1.00	78.26
ATOM	3824	CA	PRO	505	87.755	-4.660	10.097	1.00	75.62
MOTA	3825	CB	PRO	505	89.166	-4.487	10.669	1.00	75.77
MOTA	3826	CG	PRO	505	89.696	-5.884	10.715	1.00	77.07
ATOM	3827	С	PRO	505	87.709	-4.440	8.583	1.00	73.15
MOTA	3828	0	PRO	505	87.772	-3.308	8.105	1.00	72.63
ATOM	3829	N	ASN	506	87.595	-5.524	7.830	1.00	71.27
MOTA	3831	CA	ASN	506	87.518	-5.421	6.380	1.00	69.14
ATOM	3832	CB	ASN	506	88.577	-6.313	5.728	1.00	70.76
ATOM	3833	C	ASN	506	86.119	-5.840	5.940	1.00	67.30
ATOM	3834	0	ASN	506	85.834	-5.957	4.750	1.00	67.03
ATOM	3835	N	ARG	507	85.250	-6.064	6.921	1.00	65.27
ATOM	3837	CA	ARG	507	83.876	-6.479	6.669	1.00	62.86
MOTA	3838	CB	ARG	507	83.335	-7.267	7.864	1.00	65.45
ATOM	3839	С	ARG	507	82.991	-5.274	6.443	1.00	59.56
MOTA	3840	0	ARG	507	83.161	-4.247	7.100	1.00	59.70
MOTA	3841	N	VAL	508	82.057	-5.397	5.509	1.00	56.65
ATOM	3843	CA	VAL	508	81.135	-4.310	5.226	1.00	55.48
MOTA	3844	CB	VAL	508	80.850	-4.157	3.719	1.00	55.71
ATOM	3845	CG1	VAL	508	82.146	-3.962	2.962	1.00	58.18
ATOM	3846	CG2	VAL	508	80.096	-5.356	3.188	1.00	58.76
ATOM	3847	С	VAL	508	79.833	-4.537	5.979	1.00	53.10
ATOM	3848	0	VAL	508	79.352	-5.665	6.091	1.00	54.25
ATOM	3849	N	THR	509	79.282	-3.460	6.514	1.00	50.06
ATOM	3851	CA	THR	509	78.041	-3.512	7.260	1.00	45.70
MOTA	3852	CB	THR	509	78.256	-3.029	8.715	1.00	45.59
MOTA	3853	OG1	THR	509	79.395	-3.696	9.279	1.00	43.86
MOTA	3855	CG2	THR	509	77.028	-3.328	9.573	1.00	44.19
ATOM	3856	С	THR	509	77.064	-2.574	6.564	1.00	43.57
MOTA	3857	0	THR	509	77.416	-1.444	6.221	1.00	41.15
MOTA	3858	N	LYS	510	75.871	-3.073	6.268	1.00	42.96
ATOM	3860	CA	LYS	510	74.847	-2.253	5.640	1.00	41.91
ATOM	3861	CB	LYS	510	73.740	-3.144	5.091	1.00	44.74
ATOM	3862	CG	LYS	510	72.864	-2.461	4.069	1.00	51.83
MOTA	3863	CD	LYS	510	73.392	-2.645	2.659	1.00	55.00
ATOM	3864	CE	LYS	510	72.769	-3.879	2.020	1.00	58.36
MOTA	3865	NZ	LYS	510	73.069	-5.131	2.769	1.00	58.57
ATOM	3869	С	LYS	510	74.322	-1.367	6.789	1.00	40.74
MOTA	3870	0	LYS	510	73.909	-1.874	7.837	1.00	40.26
ATOM	3871	N	VAL	511	74.413	-0.052	6.624	1.00	37.21
MOTA	3873	CA	VAL	511	73.989	0.877	7. <b>6</b> 61	1.00	33.44
MOTA	3874	CB	VAL	511	75.227	1.515	8.362	1.00	34.53
ATOM	3875	CG1	VAL	511	76.100	0.436	9.014	1.00	31.98
ATOM	3876	CG2	VAL	511	76.048	2.322	7.358	1.00	34.82
MOTA	3877	С	VAL	511	73.134	1.989	7.087	1.00	31.34
ATOM	3878	0	VAL	511	73.025	2.130	5.871	1.00	31.33
MOTA	3879	N	ALA	512	72.485	2.748	7.961	1.00	30.70
MOTA	3881	CA	ALA	512	71.671	3.876	7.523	1.00	30.81

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A7	rom	3882	СВ	λ.	LA 512	_				
Α٦	MO	3883	C						06 1.00	29.85
PΑ	MO	3884	ō					24 7.9		-2.03
AT		3885	N				<del></del>	97 8.9		
AT		3887	CA	V.				6.99		
AT		3888	CB	V.			8 7.33	2 7.23		-
AT		3889	CG1							
AT		3890	CG2	VA				8 6.54		
ATO		3891	C			75.29		7 6.22		
ATO		3892	ō	VA	-	72.30		6 7.18		_
ATO		893	N	VA		71.64		4 6.16		
ATO		895	CA	LY		72.22				30.12
ATC	_	896	CB	LY		71.439		8.45		31.03
ATC		897	CG	LY		70.883	10.635		-	32.56
ATO	_	898		LY		69.977	9.516			34.31
ATO	-	899	CD	LYS		69.513	9.774			38.25
ATO		900	CE	LYS		68.514	8.719		_	47.74
ATO	_	904	NZ	LYS		67.226	8.755			51.60
ATO			C	LYS		72.357			-	58. <b>5</b> 3
ATO	_		0	LYS		73.485				30.29
ATO			N	MET	515	71.867	12.580			28.14
ATO			CA	MET	515	72.643	13.747			30.67
ATO			CB	MET	515	73.435	13.442			29.94
ATOM			CG	MET	515	72.557	13.038	5.648		30.64
ATOM			SD	MET	515	73.525	12.522	4.464	1.00	32.16
	_		CE	MET	515	74.015	10.933	3.036	1.00	37.59
ATOM			2	MET	515	71.675	14.869	3.563	1.00	29.11
ATOM		-	)	MET	515	70.462	14.664	6.635	1.00	29.71
ATOM			J	LEU	516	72.212	16.060	6.598	1.00	30.04
ATOM			CA	LEU	516	71.381	17.206	6.445	1.00	29.56
ATOM		_	B	LEU	516	72.093		6.136	1.00	30.76
ATOM		_	<b>'</b> G	LEU	516	72.396	18.508 18.724	6.526	1.00	28.20
ATOM			D1	LEU	516	73.202		8.011	1.00	28.48
ATOM				LEU	516	71.114	19.983	8.185		27. <b>5</b> 5
ATOM	392			LEU	516	71.081	18.814	8.794		25.49
ATOM	392	_	:	LEU	516	71.728	17.225	4.647	1.00	30.97
ATOM	392		;	LYS	517	70.030	16.534	3.851	1.00	29.93
ATOM	392	6 C	<b>A</b> 1	LYS	517	69.677	17.946	4.291	1.00	31.57
ATOM	392		В ј	LYS	517	68.169	18.117	2.899	1.00	31.44
ATOM	392		3 1	LYS	517	67.375	18.310	2.752		34.79
ATOM	392		) I	LYS	517	66.148	17.098	3.194	1.00	88.42
ATOM	393	O CE	e i	YS	517	65.087	16.888	2.343	1.00 4	6.52
ATOM	393	1 N2		YS	517	63.901	17.950	2.582	1.00 5	3.77
ATOM	393	5 C	L	YS	517	70.457	17.740	1.690		6.38
ATOM	3936			YS	517	70.437	19.377	2.499		0.18
ATOM	3931	7 N		ER	518	70.646	20.134	3.370		7.47
ATOM	3939	CA		ER	518		19.594	1.201		1.13
ATOM	3940	CB		ER	518	71.394	20.747	0.693		2.11
ATOM	3941			ER	518	71.518	20.652	-0.824		3.45
ATOM	3943		_	ER	518	70.242	20.567		_	4.51
ATOM	3944					70.814	22.103	_		2.81
ATOM	3945				518 510	71.515	23.123			4.03
ATOM	3947				519 510	69.540	22.117			9.80
ATOM	3948			_	519	68.886	23.354			3.94
ATOM	3949		AS		519 510	67.473	23.421			3.90
			AS	. <del>.</del> .	519	66.542	22.332			42

66.542 22.332 1.771 1.00 34.42

SSSD/55145. v01

MOTA	3950	OD1	ASP	519	67.020	21.328	2.333	1.00	35.58
ATOM	3951	OD2	ASP	519	65.313	22.485	1.617	1.00	41.83
ATOM	3952	С	ASP	519	68.829	23.559	3.342	1.00	29.08
MOTA	3953	0	ASP	519	68.177	24.485	3.816	1.00	29.79
MOTA	3954	N	ALA	520	69.514	22.710	4.099	1.00	29.73
ATOM	3956	CA	ALA	520	69.488	22.824	5.558	1.00	29.16
MOTA	3957	СВ	ALA	520	70.174	21.639	6.190	1.00	28.13
ATOM	3958	С	ALA	520	70.122	24.108	6.040	1.00	28.06
ATOM	3959	0	ALA	520	70.880	24.741	5.309	1.00	28.84
MOTA	3960	N	THR	521	69.800	24.491	7.272	1.00	27.84
ATOM	3962	CA	THR	521	70.357	25.692	7.885	1.00	30.45
ATOM	3963	СВ	THR	521	69.254	26.635	8.463	1.00	33.56
ATOM	3964	OG1	THR	521	68.547	25.968	9.520	1.00	36.27
ATOM	3966	CG2	THR	521	68.275	27.074	7.379	1.00	36.06
ATOM	3967	С	THR	521	71.251	25.263	9.048	1.00	30.04
ATOM	3968	0	THR	521	71.348	24.072	9.369	1.00	28.16
MOTA	3969	N	GLU	522	71.876	26.241	9.696	1.00	31.42
ATOM	3971	CA	GLU	522	72.745	25.978	10.832	1.00	36.94
ATOM	3972	CB	GLU	522	73.404	27.282	11.299	1.00	44.74
ATOM	3973	CG	GLU	522	74.414	27.130	12.450	1.00	58.34
ATOM	3974	CD	GLU	522	75.769	26.579	12.009	1.00	64.50
ATOM	3975	OE1	GLU	522	76.798	27.261	12.231	1.00	64.89
ATOM	3976	OE2	GLU	522	75.806	25.461	11.452	1.00	70.26
ATOM	3977	C	GLU	522	71.932	25.345	11.969	1.00	34.02
ATOM	3978	0	GLU	522	72.428	24.480	12.684	1.00	31.11
ATOM	3979	N	LYS	523	70.670	25.750	12.007	1.00	32.53
ATOM	3981	CA	LYS	523	69.805	25.730	13.135	1.00	34.06
ATOM	3982	CB	LYS	523	68.481	25.210	13.188	1.00	39.54
ATOM	3983	CG	LYS	523	67.560	25.541	14.322	1.00	45.55
ATOM	3984	CD	LYS	523	66.360	24.776	13.789	1.00	52.08
ATOM	3985	CE	LYS	523	65.443	24.312	14.914	1.00	54.16
ATOM	3986	NZ	LYS	523	64.313	23.509	14.373	1.00	54.38
ATOM	3990	C	LYS	523	69.572	23.733	12.861	1.00	31.73
MOTA	3991	0	LYS	523	69.589	22.922	13.788	1.00	31.15
ATOM	3992	N	ASP	524	69.374	23.383	11.590	1.00	29.22
ATOM	3994	CA	ASP	524	69.182	21.980	11.214	1.00	28.79
ATOM	3995	CB	ASP	524	68.928	21.831	9.714	1.00	27.65
ATOM	3996	CG	ASP	524	67.586	22.396	9.286	1.00	33.89
ATOM	3997	OD1	ASP	524	66.568	22.106	9.954	1.00	34.66
MOTA	3998	OD2	ASP	524	67.549	23.120	8.270	1.00	30.04
ATOM	3999	С	ASP	524	70.424	21.190	11.606	1.00	28.00
ATOM	4000	0	ASP	524	70.317	20.104	12.162	1.00	30.83
ATOM	4001	N	LEU	525	71.603	21.761	11.347	1.00	29.87
ATOM	4003	CA	LEU	525	72.873	21.121	11.700	1.00	27.60
ATOM	4004	CB	LEU	525	74.064	21.997	11.282	1.00	24.08
ATOM	4005	CG	LEU	525	75.462	21.433	11.593	1.00	26.11
ATOM	4006	CD1	LEU	525	75.597	19.979	11.098	1.00	23.67
ATOM	4007	CD2	LEU	525	76.530	22.321	10.967	1.00	21.28
ATOM	4008	C	LEU	525	72.909	20.869	13.200	1.00	26.38
ATOM	4009	0	LEU	525	73.249	19.777	13.653	1.00	26.09
ATOM	4010	N	SER	526	72.560	21.902	13.956	1.00	29.72
ATOM	4012	CA	SER	526	72.500	21.861	15.422	1.00	32.16
ATOM	4013	CB	SER	526	71.980	23.209	15.939	1.00	33.45
ATOM	4014	OG	SER	526	71.793	23.213	17.343	1.00	40.42
			~=		12.123		11.343	1.00	40.42

3 moss			
ATOM 4016		26 71 572	
ATOM 4017	_		20.728 15.902 1.00 31.64
ATOM 4018	NT no.		20,030 16 000
ATOM 4020	C2	,0.434	20.561 15 200 32.54
ATOM 4021	CD	69.492	19.527 15.524
ATOM 4022		<sup>27</sup> 68.187	19 767
ATOM 4023		27 67.418	14.765 1.00 29 35
	OD1 ASP 52	67.759	13.2/8 1.00 31 37
3.000	OD2 ASP 52	66.456	<sup>21.549</sup> 16.353 1 00 3
ATOM 4025	C ASP 52	00.436	21.369 14.591 1 00 33
ATOM 4026	O ASP 52	,0.036	18.131 15 246
ATOM 4027	NI	97.034	17.212 16 045
ATOM 4029	C3		17.962 14 120 29.65
ATOM 4030	CD	302	16 660 29.29
ATOM 4031	CB LEU 52	<sup>8</sup> 71.780	- + +·00 /9 QA
3	CG LEU 528	72.315	12.336 1.00 26 45
	CD1 LEU 528	71.240	15.276 11.840 1.00 22 -
_	CD2 LEU 528		14.189 12.035 1 00 05
ATOM 4034	C LEU 528	. • . , 50	15.387 10.370
ATOM 4035	^	, 2 , 44 7	16.319 14 776
ATOM 4036	NT	- 2.01/	15.162 15 170 29.72
ATOM ADD	CD 229	73.224	17 220 25 28.98
ATOM	329	74.305	17 121 30.15
ATOM AS A	CB ILE 529	75.188	10.134 1.00 28 80
ATOM 4045	CG2 ILE 529	76.175	16.268 1.00 26 91
ATOM 10:-	CG1 ILE 529	75.960	17.423 1.00 24 02
	CD1 ILE 529	76.663	10.613 14.984 1 00
	ILE 529	77	19.932 14.973 1.00 22
ATOM 4044 C			16.799 17.518 1 00 20
ATOM 4045 N		74.172	15.880 70.702
ATOM 4047 C	221 230	72.672	17.524 17.006
ATOM 4048 C			17 247 26.84
ATOM AGAS	221 230	7.0	19 251 1-00 31.46
ATION	<b>521</b> 530	~ .	19.521 1.00 36 17
ATOM 407-	SER 530		18.431 1.00 47 59
	SER 530		15.822 19.248 1 00
Ti Mana	GLU 531	70	.5.136 20.270 1 00 20 -
ATOM 4055 CA	GLU 531		.5.357 18.132 1 00 27 -
ATOM 4056 CB		70.458 1	3.999 10.000
ATOM 4057 CG	020 531	69.709 <sub>1</sub>	3.727 16 700 28.71
ATOM 4058 CD	920 931	69.147 1	2.319 16 727
ATOM 4059 OE	1 20 331	68.510 1	1.979 15 41.
ATOM 100	450 331	·	+.00 {{ gp
ATOM	0 221		13.281 1.00 37 60
ATOM 4000	GLU 531	7.	14.510 1.00 34 70
3.00	GLU 531		112/4 18.271 1 nn nn -
ATOM 4063 N	MET 532		2.007 19.019 1 00 05
ATOM 4065 CA	MET 532	72.686 13	17.567 1 00 00
ATOM 4066 CB		73.851 12	296 17 545
ATOM 4067 CG		74.948 12	.786 76 600
ATOM	MET 532		117 15 27.41
ATOM 40 ==	MET 532		675 16.872 1.00 26.71
ATOM	MET 532		·6/3 15.640 1.00 32 27
3.000	MET 532		.400 16.117 1 00 24 15
ATOM 4071 O	MET 532	74.389 12.	.280 19.078 1 00 22
ATOM 4072 N		74.700 11.	230 19 530
ATOM 4074 CA		74.481 13	454 10 555
ATOM 4075 CB	GLU 533	74.985 13.	546 21 022
ATOM 100	GLU 533		008 31 433 1.00 29.66
ATOM 10==	GLU 533		507 21.423 1.00 32.23
ATOM 4077 CD	GLU 533		20.651 1.00 34 47
CCCD 15-		77.656 14.	937 20.774 1.00 38.03
SSSD/55145 v01			20.03

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ATOM	4078	OE1	GLU	533	78.168	14.780	21.903	1.00	39.75	
ATOM	4079	OE2	GLU	533	78.192	14.497	19.736	1.00	38.75	
MOTA	4080	С	GLU	533	74.058	12.815	22.005	1.00	31.55	
MOTA	4081	0	GLU	533	74.521	12.083	22.889	1.00	30.63	
MOTA	4082	N	MET	534	72. <b>7</b> 50	12.958	21.799	1.00	31.31	
MOTA	4084	CA	MET	534	71.789	12.289	22.664	1.00	30.78	
MOTA	4085	CB	MET	534	70.348	12.672	22.319	1.00	31.23	
MOTA	4086	CG	MET	534	69.453	12.648	23.551	0.50	29.35 PR	Tl
ATOM	4087	SD	MET	534	67.688	12.563	23.246	0.50	28.79 PR	Tl
ATOM	4088	CE	MET	534	67.290	14.230	22.875	0.50	26.96 PR	Tl
ATOM	4089	С	MET	534	71.991	10.773	22.560	1.00	28.82	
MOTA	4090	0	MET	534	72.053	10.083	23.568	1.00	30.10	
ATOM	4091	N	MET	535	72.149	10.271	21.339	1.00	29.16	
ATOM	4093	CA	MET	535	72.381	8.852	21.110	1.00	29.37	
ATOM	4094	CB	MET	535	72.546	8.551	19.617	1.00	27.35	
ATOM	4095	CG	MET	535	71.281	8.790	18.817	1.00	28.40	
ATOM	4096	SD	MET	535	71.255	7.955	17.255	1.00	30.26	
MOTA	4097	CE	MET	535	71.336	9.279	16.188	1.00	35.50	
MOTA	4098	C	MET	535	73.612	8.388	21.887	1.00	30.36	
MOTA	4099	0	MET	535	73.626	7.287	22.460	1.00	26.13	
ATOM	4100	N	LYS	536	74.640	9.233	21.909	1.00	30.70	
ATOM	4102	CA	LYS	536	75.850	8.913	22.649	1.00	31.76	
ATOM	4103	CB	LYS	536	76.934	9.954	22.388	1.00	31.05	
MOTA	4104	CG	LYS	536	77.550	9.883	21.004	1.00	26.80	
ATOM	4105	CD	LYS	536	78.534	11.017	20.860	1.00	31.05	
ATOM	4106	CE	LYS	536	79.132	11.138	19.466	1.00	29.83	
ATOM	4107	NZ	LYS	536	79.957	12.377	19.440	1.00	29.32	
MOTA	4111	С	LYS	536	75.550	8.834	24.150	1.00	31.99	
ATOM	4112	0	LYS	536	75.920	7.859	24.806	1.00	31.92	
MOTA	4113	N	MET	537	74.837	9.826	24.676	1.00	31.81	
MOTA	4115	CA	MET	537	74.517	9.835	26.090	1.00	35.37	
ATOM	4116	CB	MET	537	73.860	11.154	26.506	1.00	41.32	
MOTA	4117	CG	MET	537	74.828	12.335	26.610	1.00	51.50	
ATOM	4118	SD	MET	537	76.234	12.090	27.776	1.00	57.48	
MOTA	4119	CE	MET	537	75.460	12.637	29.334	1.00	56.91	
ATOM	4120	C	MET	537	73.630	8.679	26.499	1.00	36.11	
MOTA	4121	0	MET	537	73.845	8.084	27.548	1.00	38.54	
MOTA	4122	N	ILE	538	72.652	8.347	25.661	1.00	33.69	
ATOM	4124	CA	ILE	538	71.704	7.277	25.954	1.00	31.62	
MOTA	4125	CB	ILE	538	70.492	7.314	24.974	1.00	28.21	
ATOM	4126	CG2	ILE	538	69.681	6.013	25.034	1.00	28.22	
ATOM	4127	CG1	ILE	538	69.590	8.488	25.338	1.00	23.74	
MOTA	4128	CD1	ILE	538	68.487	8.728	24.344	1.00	27.94	
ATOM	4129	С	ILE	538	72.322	5.894	26.008	1.00	31.07	
ATOM	4130	0	ILE	538	71.952	5.080	26.860	1.00	33.13	
ATOM	4131	N	GLY	539	73.239	5.611	25.094	1.00	29.52	
ATOM	4133	CA	GLY	539	73.871	4.309	25.093	1.00	28.40	
ATOM	4134	С	GLY	539	73.111	3.275	24.289	1.00	30.21	
MOTA	4135	0	GLY	539	72.018	3.554	23.788	1.00	29.66	
MOTA	4136	N	LYS	540	73.679	2.074	24.199	1.00	28.44	
MOTA	4138	CA	LYS	540	73.105	0.984	23.426	1.00	31.09	
MOTA	4139	CB	LYS	540	74.215	0.089	22.895	1.00	33.15	
MOTA	4140	CG	LYS	540	75.116	0.776	21.906	1.00	39.54	
ATOM	4141	CD	LYS	540	76.125	-0.175	21.329	1.00	43.98	

	rom 4	142 (	CE I	YS 5	40	77.03						
		143 1			40	76.33		. 562	-0.5		00	50.79
			C L		40	72.05		.977			00	51.09
		L48. (		_	40	72.03		.087			00	32.78
		.49 N	1 н		41	72.08		.195			00	32.41
AT	OM 41	51 (			41			. 374			00	31.20
AT		.52 C			11	70.08 68.91		.304	23.59		00	31.53
AT		53 C		IS 54		67.948		. 630	24.29	98 1.0		30.69
ATO		54 C		IS 54		67.938		613	24.88		00	31.18
ATO		55 N	Di H	_		66.882		255	26.07		0	33.02
ATO		57 C	E1 H)			66.268	-	123	24.16		0	30.56
ATO		58 ท	E2 H1			66.886		037	24.88		0	32.95
ATC		50 C	HI			69.590		140	26.05		0	31.79
ATC		51 0	HI					013	22.34		0	32.72
ATO	M 416	52 N	LY			69.495			21.27		0	30.34
ATO	M 416	4 C				69.282			22.47		0	32.32
ATO		5 CE				68.828 68.637			21.359		0	30.29
ATO	•	6 C	LY			67.560	-5.		21.798		0	29.34
ATO		7 0	LY			67.369	-3.6		20.692		0	29.09
ATO		8 N	ASI			66.683	-3.9		19.507			29.12
ATO		0 CA				65.425	-3.0		21.446			28.54
ATO		1 CB				64.245	-2.5		20.869			29.10
ATON						64.253	-3.0		21.712		) ;	29.69
ATOM		3 OD:				64.510	-4.5		21.900			29.62
ATOM		ND:				64.020	-5.0		23.000			31.63
ATOM		7 C	ASN			65.299	-5.2		20.828	1.00	7	28.66
ATOM		_	ASN			64.207	-1.0		20.532	1.00	2	9.61
ATOM	-	N	ILE			66.432	-0.5		20.578	1.00		8.00
ATOM			ILE			66.466	-0.4		20.222	1.00		8.39
ATOM			ILE			66.903	0.9		19.804	1.00	2	5.73
ATOM		CG2	ILE	544		66.083	1.9		20.935	1.00	2	5.98
ATOM	4184	CG1	ILE	544		68.412	1.72 1.86		22.215	1.00	2	2.04
ATOM	4185		ILE	544		68.901	2.84		21.209	1.00		4.30
ATOM	4186	C	ILE	544		67.463	1.02		22.274	1.00		2.83
ATOM	4187	0	ILE	544		68.276	0.10		18.639	1.00		6.20
ATOM	4188	N	ILE	545		67.307	2.01		18.467	1.00		5.46
ATOM	4190	CA	ILE	545		68.223	2.20		17.771	1.00		5.26
ATOM ATOM	4191	CB	ILE	545		67.647	3.19		16.641	1.00		7.62
ATOM	4192	CG2	ILE	545		68.726	3.59		15.585	1.00	28	3.33
	4193	CG1	ILE	545		66.453	2.56	_	4.562	1.00		3.00
ATOM	4194	CD1	ILE	545		66.850	1.46		4 . 856	1.00		.69
ATOM ATOM	4195	C	ILE	545		69.492	2.79		3.875	1.00		.17
ATOM	4196	0	ILE	545		69.468	3.872		7.267 7.846	1.00		.23
	4197	N	ASN	546		70.595	2.069		7.164	1.00		.97
ATOM	4199	CA	ASN	546		71.845	2.508		7.774	1.00		.45
ATOM	4200	CB	ASN	546		72.580	1.309			1.00		.58
ATOM	4201	CG	ASN	546		71.812	0.673		8.384	1.00		. 34
ATOM	4202	OD1	ASN	546		71.634	1.277		9.527	1.00		.52
ATOM	4203	ND2	ASN	546		71.341	-0.542			1.00		. 82
ATOM	4206	C	ASN	546		72.810	3.264			1.00		. 57
ATOM	4207	0	ASN	546		72.858	3.264		-	1.00	28.	
MOTA	4208	N	LEU	547		73.578	4.155		_	1.00	29.	
MOTA	4210	CA	LEU	547		4.618	4.936			1.00	29.	
MOTA	4211	CB	LEU	547		5.075	6.081			1.00	30.	
						- · · · <del>-</del>	0.001	1	7.745	1.00	25.	85

ATOM	4212	CG	LEU	547	76.161	7.034	17.232	1.00	27.73	
MOTA	4213	CD1	LEU	547	75.670	7.851	16.033	1.00	27.38	
MOTA	4214	CD2	LEU	547	76.545	7.966	18.345	1.00	29.14	
ATOM	4215	С	LEU	547	75.811	4.004	16.567	1.00	32.22	
ATOM	4216	0	LEU	547	76.256	3.291	17.471	1.00	33.38	
ATOM	4217	N	LEU	548	76.317	4.005	15.335	1.00	32.12	
ATOM	4219	CA	LEU	548	77.452	3. <b>1</b> 59	14.960	1.00	32.94	
MOTA	4220	CB	LEU	548	77.103	2.310	13.740	1.00	29.97	
MOTA	4221	CG	LEU	548	75.839	1.458	13.840	1.00	31.55	
ATOM	4222	CD1	LEU	548	75.662	0.713	12.540	1.00	27.85	
ATOM	4223	CD2	LEU	548	75.917	0.500	15.025	1.00	26.34	
ATOM	4224	С	LEU	548	78.726	3.955	14.654	1.00	36.06	
ATOM	4225	0	LEU	548	79.836	3.410	14.668	1.00	36.42	
ATOM	4226	N	GLY	549	78.562	5.219	14.298	1.00	35.78	
MOTA	4228	CA	GLY	549	79.713	6.042	13.987	1.00	36.22	
MOTA	4229	C	GLY	549	79.267	7.376	13.433	1.00	35.30	
ATOM	4230	0	GLY	549	78.062	7.646	13.362	1.00	33.46	
ATOM	4231	N	ALA	550	80.232	8.206	13.042	1.00	34.94	
MOTA	4233	CA	ALA	550	79.945	9.525	12.490	1.00	31.91	
MOTA	4234	CB	ALA	550	79.588	10.495	13.613	1.00	30.54	
ATOM	4235	С	ALA	550	81.128	10.077	11.715	1.00	31.58	
MOTA	4236	0	ALA	550	82.281	9.832	12.080	1.00	31.23	
ATOM	4237	N	CYS	551	80.818	10.812	10.643	1.00	31.13	
ATOM	4239	CA	CYS	551	81.805	11.503	9.804	1.00	28.28	
MOTA	4240	CB	CYS	551	81.621	11.180	8.316	1.00	27.27	
MOTA	4241	SG	CYS	551	81.771	9.449	7.839	1.00	30.33	
ATOM	4242	С	CYS	551	81.450	12.960	10.074	1.00	25.88	
ATOM	4243	0	CYS	551	80.432	13.458	9.605	1.00	27.73	
MOTA	4244	N	THR	552	82.214	13.586	10.954	1.00	25.35	
MOTA	4246	CA	THR	552	81.988	14.967	11.353	1.00	26.79	
ATOM	4247	CB	THR	552	82.051	15.092	12.899	1.00	27.76	
MOTA	4248	OG1	THR	552	83.392	14.839	13.338	1.00	27.62	
ATOM	4250	CG2	THR	552	81.119	14.086	13.575	1.00	29.17	
ATOM	4251	С	THR	552	83.036	15.931	10.790	1.00	25.03	
ATOM	4252	0	THR	552	82.825	17.137	10.746	1.00	25.34	
ATOM	4253	N	GLN	553	84.174	15.385	10.381	1.00	27.34	
ATOM	4255	CA	GLN	553	85.285	16.190	9.888	1.00	26.31	
ATOM	4256	CB	GLN	553	86.601	15.639	10.468	1.00	25.05	
ATOM	4257	CG	GLN	553	86.581	15.491	11.993		24.78	
ATOM	4258	CD	GLN	553	86.382	16.823	12.709	1.00	25.40	
MOTA	4259	OE1	GLN	553	87.175	17.748	12.546	1.00	33.74	
ATOM	4260	NE2	GLN	553	85.338	16.920	13.516	1.00	25.61	
ATOM	4263	C	GLN	553	85.390	16.274	8.379	1.00	27.08	
ATOM	4264	0	GLN	553	85.083	15.318	7.669	1.00	28.76	
ATOM ATOM	4265	N	ASP	554	85.804	17.438	7.899	1.00	28.63	
	4267	CA	ASP	554	86.015	17.677	6.471	1.00	29.70	
ATOM	4268	CB	ASP	554	87.335	17.050	6.051	1.00	29.73	
ATOM	4269	CG	ASP	554	88.480	17.587	6.857	1.00	33.38	
ATOM	4270	OD1	ASP	554	88.794	18.780	6.711	1.00	36.53	
MOTA	4271	OD2	ASP	554	89.024	16.841	7.687	1.00	36.40	
ATOM	4272	C	ASP	554	84.908	17.258	5.522	1.00	29.64	
MOTA	4273	0	ASP	554	85.112	16.422	4.643	1.00	32.06	
ATOM	4274	N	GLY	555	83.748	17.881	5.679	1.00	28.59	
ATOM	4276	CA	GLY	555	82.620	17.579	4.825	1.00	26.85	



ATC		77 C	GL	Y 555	81.333	17.43	4 5 600	<b>.</b>	
ATO		_	GL	Y 555	81.319				
ATO	M 427	79 N	PR	0 556	80.229	-/.55			
ATO	M 428	0 CD	PR	0 556	80.159				
ATO		1 CA	PR	0 556	78.920				
ATO	M 428	2 CB	PRO		78.033				
ATO		3 CG			79.025				23.37
ATO	M 428	4 C	PRO		78.885				24.44
ATO	M 428	5 0	PRO		79.515				26.50
ATON	428	6 N	LEC		78.171	14.875			27.38
ATON	428	8 CA	LEU		78.032	16.314		_	26.25
ATON	428	9 CB	LEU		77.403	15.452		1.00	28.25
ATOM	1 429	O CG	LEU	_	76.922	16.217		1.00	27.09
ATOM	1 429	L CD1			78.088	15.414		1.00	28.35
ATOM				-		14.733		1.00	25.54
ATOM	4293		LEU		76.204	16.340	12.271	1.00	26.91
ATOM			LEU	_	77.169	14.246	8.554	1.00	29.06
ATOM			TYR		76.060	14.385	8.011	1.00	29.05
ATOM			TYR		77.717	13.065	8.807	1.00	29.43
ATOM			TYR		77.018	11.823	8.573	1.00	28.02
ATOM			TYR		77.813	10.918	7.632	1.00	27.83
ATOM				558 550	77.969	11.414	6.203	1.00	31.70
ATOM				558 558	78.966	10.893	5.383	1.00	32.90
ATOM	4302			558	79.121	11.315	4.073	1.00	32.69
ATOM	4303		TYR	558	77.122	12.386	5.666	1.00	30.23
ATOM	4304	CZ	TYR	558	77.271	12.815	4.350	1.00	29.97
ATOM	4305	OH	TYR	558	78.280	12.272	3.560	1.00	33.20
ATOM	4307	C	TYR	558	78.452	12.681	2.253	1.00	35.32
ATOM	4308		TYR	558	76.848	11.131	9.932	1.00	28.42
ATOM	4309	O N	TYR	558	77.823	10.902	10.647	1.00	27.81
ATOM	4311		VAL	559	75.601	10.870	10.313	1.00	29.20
ATOM	4312	CA	VAL	559	75.286	10.175	11.564	1.00	29.17
ATOM	4312	CB	VAL	559	74.102	10.832	12.329	1.00	28.53
ATOM	4314	CG1	VAL	559	73.802	10.036	13.607	1.00	27.08
ATOM	4315	CG2	VAL	559	74.456	12.281	12.687	1.00	23.27
ATOM		C	VAL	559	74.911	8.772	11.137		26.41
ATOM	4316	0	VAL	559	73.834	8.536	10.593		25.91
ATOM	4317 4319	N ~~	ILE	560	75.824	7.846	11.371		26.71
ATOM	4319	CA	ILE	560	75.638	6.465	10.966		27.55
ATOM	4321	CB	ILE	560	77.012	5.829	10.619		28.48
ATOM		CG2	ILE	560	76.819	4.468	9.979		29.18
ATOM	4322	CG1	ILE	560	77.793	6.745	9.657		27.99
ATOM	4323	CD1	ILE	560	79.274	6.399	9.525		27.99 28.97
	4324	C	ILE	560	74.917	5.644	12.034		
MOTA	4325	0	ILE	560	75.404	5.497	13.160		29.17
ATOM	4326	N	VAL	561	73.743	5.129			28.92
ATOM	4328	CA	VAL	561	72.957	4.325			28.60
ATOM	4329	CB	VAL	561	71.634	5.061			28.58
ATOM	4330	CG1	VAL	561	71.951	6.400			27.53
ATOM	4331	CG2	VAL	561	70.697	5.246			22.44
ATOM	4332	C	VAL	561	72.618	2.956			3.19
ATOM	4333	0	VAL	561	72.875	_			8.20
ATOM	4334	N	GLU	562	72.057				7.99
ATOM	4336	CA	GLU	562	71.666				9.17
ATOM	4337	CB		562	71.199			_	8.96
						-0.086	13.589	1.00 2	7.34

ATOM	4338	CG	GLU	562	72.308	-0.331	14.583	1.00	30.12
MOTA	4339	CD	GLU	562	71.838	-1.075	15.808	1.00	32.29
ATOM	4340	OE1	GLU	562	72.526	-2.030	16.217	1.00	32.45
MOTA	4341	OE2	GLU	562	70.785	-0.702	16.362	1.00	30.16
ATOM	4342	С	GLU	562	70.580	0.794	11.340	1.00	29.79
ATOM	4343	0	GLU	562	69.690	1.653	11.386	1.00	29.75
ATOM	4344	N	TYR	563	70.684	-0.106	10.369	1.00	30.51
ATOM	4346	CA	TYR	563	69.735	-0.209	9.267	1.00	33.76
ATOM	4347	CB	TYR	563	70.494	-0.602	7.988	1.00	31.04
ATOM	4348	CG	TYR	563	69.624	-0.928	6.806	1.00	33.40
ATOM	4349	CD1	TYR	563	68.693	-0.019	6.340	1.00	33.07
ATOM	4350	CE1	TYR	563	67.908	-0.301	5.240	1.00	34.71
ATOM	4351	CD2	TYR	563	69.749	-2.141	6.147	1.00	34.61
ATOM	4352	CE2	TYR	563	68.970		5.035	1.00	36.54
MOTA	4353	CZ	TYR	563	68.047	-1.518	4.589	1.00	36.83
ATOM	4354	OH	TYR	563	67.261	-1.805	3.501	1.00	38.81
ATOM	4356	С	TYR	563	68.655	-1.269	9.588	1.00	36.14
MOTA	4357	0	TYR	563	68.946	-2.365	10.023	1.00	37.70
MOTA	4358	N	ALA	564	67.406	-0.948	9.309	1.00	37.87
MOTA	4360	CA	ALA	564	66.276	-1.832	9.534	1.00	38.49
ATOM	4361	CB	ALA	564	65.278	-1.167	10.458	1.00	42.57
ATOM	4362	С	ALA	564	65.645	-2.153	8.179	1.00	39.65
ATOM	4363	0	ALA	564	64.796	-1.423	7.687	1.00	39.74
ATOM	4364	N	SER	565	66.039	-3.280	7.607	1.00	40.06
ATOM	4366	CA	SER	565	65.567	-3.699	6.295	1.00	40.67
ATOM	4367	CB	SER	565	66.267	-4.986	5.883	1.00	38.71
ATOM	4368	OG	SER	565	66.107	-5.964	6.889	1.00	41.35
ATOM	4370	С	SER	565	64.081	-3.884	6.106	1.00	42.17
ATOM	4371	0	SER	565	63.585	-3.741	4.992	1.00	44.25
ATOM	4372	N	LYS	566	63.360	-4.207	7.167	1.00	41.71
ATOM	4374	CA	LYS	566	61.928	-4.427	7.015	1.00	40.22
ATOM	4375	CB	LYS	566	61.525	-5.668	7.800	1.00	39.51
MOTA	4376	CG	LYS	566	62.202	-6.910	7.226	1.00	41.48
MOTA	4377	CD	LYS	566	62.113	-8.094	8.149	1.00	41.53
MOTA	4378	CE	LYS	566	62.710	-9.312	7.491	1.00	41.18
ATOM	4379	NZ	LYS	566	62.763	-10.458	8.438	1.00	46.17
ATOM	4383	С	LYS	566	61.007	-3.220	7.263	1.00	40.47
ATOM	4384	0	LYS	566	59.800	-3.367	7.486	1.00	42.68
MOTA	4385	N	GLY	567	61.584	-2.026	7.167	1.00	38.90
ATOM	4387	CA	GLY	567	60.826	-0.799	7.336	1.00	37.13
ATOM	4388	С	GLY	567	60.199	-0.592	8.694	1.00	36.72
ATOM	4389	0	GLY	567	60.644	-1.172	9.683	1.00	38.48
ATOM	4390	N	ASN	568	59.191	0.273	8.753	1.00	35.77
ATOM	4392	CA	ASN	568	58.518	0.549	10.015	1.00	35.36
ATOM	4393	CB	ASN	568	57.883	1.957	10.045	1.00	36.30
MOTA	4394	CG	ASN	568	56.635	2.088	9.169	1.00	38.06
MOTA	4395	OD1	ASN	568	55.623	1.421	9.383	1.00	38.66
ATOM	4396	ND2	ASN	568	56.686	3.010	8.221	1.00	37.29
ATOM	4399	С	ASN	568	57.504	-0.532	10.341	1.00	33.04
ATOM	4400	0	ASN	568	57.061	-1.265	9.461	1.00	32.10
ATOM	4401	N	LEU	569	57.142	-0.612	11.617	1.00	33.59
ATOM	4403	CA	LEU	569	56.199	-1.604	12.132	1.00	32.91
MOTA	4404	CB	LEU	569	56.045	-1.428	13.647	1.00	33.84
ATOM	4405	CG	LEU	569	55.088	-2.343	14.403	1.00	31.96
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**ATOM** 4406 CD1 LEU 569 55.522 -3.797 14.216 1.00 33.20 ATOM 4407 CD2 LEU 569 55.089 -1.967 15.868 30.81 1.00 ATOM 4408 C LEU 569 54.820 -1.591 11.478 1.00 32.12 MOTA 4409 0 LEU 569 54.214 -2.645 11.300 1.00 33.08 MOTA 4410 N ARG 570 54.315 -0.409 11.148 1.00 32.05 MOTA 4412 CA ARG 570 52.999 -0.293 10.529 1.00 35.21 ATOM 4413 CB ARG 570 52.659 1.173 10.256 1.00 36.77 ATOM 4414 CG ARG 570 51.282 1.370 9.653 1.00 43.11 ATOM 4415 CD ARG 570 51.203 2.690 8.926 1.00 49.24 MOTA 4416 NE ARG 570 52,154 2.775 7.815 1.00 55.77 MOTA 4418 CZARG 570 52.995 3.790 7.619 1.00 58.89 MOTA 4419 NH1 ARG 570 53.016 4.820 8.463 1.00 61.61 ATOM 4422 NH2 ARG 570 53.804 3.786 6.566 1.00 59.16 ATOM 4425 C ARG 570 52.992 -1.063 9.220 1.00 35.16 ATOM 4426 0 ARG 570 52.145 -1.922 8.990 1.00 35.50 **ATOM** 4427 N GLU 571 53.971 -0.760 8.383 1.00 36.29 MOTA 4429 CA GLU 571 54.111 -1.400 7.089 1.00 37.51 **ATOM** 4430 CB GLU 571 55.219 -0.701 6.308 1.00 41.27 ATOM 4431 CG GLU 571 54.945 0.778 6.110 1.00 49.88 ATOM 4432 CD GLU 571 56.087 1.516 5.436 1.00 57.58 **ATOM** 4433 OE1 GLU 571 57.264 1.122 5.636 1.00 60.59 **ATOM** 4434 OE2 GLU 571 55.804 2.504 4.714 1.00 61.14 MOTA 4435 C GLU 571 54.399 -2.896 7.228 1.00 36.24 ATOM 4436 O GLU 571 53.889 -3.716 6.459 1.00 34.22 ATOM 4437 N TYR 572 55.202 -3.238 8.232 1.00 35.98 **ATOM** 4439 CA TYR 572 55.570 -4.619 8.517 1.00 35.34 ATOM 4440 CB TYR 572 56.526 -4.656 9.714 1.00 30.94 ATOM 4441 CG TYR 572 56.959 -6.034 10.180 1.00 32.71 MOTA 4442 CD1 TYR 572 58.009 -6.714 9.547 1.00 32.33 ATOM 4443 CE1 TYR 572 58.464 -7.940 10.026 1.00 30.31 MOTA 4444 CD2 TYR 572 56.369 -6.626 11.303 1.00 33.43 4445 MOTA CE2 TYR 572 56.813 -7.851 11.791 1.00 31.46 MOTA 4446 CZTYR 572 57.864 -8.502 11.148 1.00 33.99 ATOM, 4447 OH TYR 572 58.311 -9.706 11.640 1.00 36.30 **ATOM** 4449 C TYR 572 54.312 -5.425 8.826 1.00 37.26 **ATOM** 4450 0 TYR 572 54.121 -6.530 8.314 1.00 36.91 ATOM 4451 N LEU 573 53.457 -4.850 9.665 1.00 36.82 ATOM 4453 CA LEU 573 52.208 -5.476 10.075 1.00 35.56 ATOM 4454 CB LEU 573 51.537 -4.629 11.165 1.00 34.03 ATOM 4455 CG LEU 573 52.238 -4.527 12.519 1.00 32.82 ATOM 4456 CD1 LEU 573 51.621 -3.423 13.377 1.00 28.95 **ATOM** 4457 CD2 LEU 573 52.168 -5.858 13.207 1.00 29.46 ATOM 4458 С LEU 573 51.237 -5.658 8.915 1.00 34.56 **ATOM** 4459 0 LEU 573 50.670 -6.729 8.726 1.00 34.80 ATOM 4460 N GLN 574 51.030 -4.602 8.150 1.00 37.10 ATOM 4462 CA GLN 574 50.101 -4.666 7.031 1.00 41.15 ATOM 4463 CB GLN 574 49.875 -3.278 6.457 1.00 41.63 ATOM 4464 CG GLN 574 49.089 -2.375 7.366 1.00 43.13 ATOM 4465 CD GLN 574 49.063 -0.959 6.860 1.00 47.77 ATOM 4466 OE1 GLN 574 49.655 -0.647 5.827 1.00 50.00 **ATOM** 4467 NE2 GLN 574 48.378 -0.086 7.582 1.00 49.67 ATOM 4470 C GLN 574 50.529 -5.627 5.934 1.00 42.38 ATOM 4471 0 GLN 574 49.685 -6.284 5.318 1.00 44.56

SSSD/55145. v01

4472

N

ALA

575

51.835

-5.717

5.697

1.00

41.99

ATOM

ATOM	4474	CA	ALA	575	52.367	-6.608	4.676	1.00	41.29
MOTA	4475	CB	ALA	575	53.841	-6.325	4.446	1.00	40.43
MOTA	4476	C	ALA	575	52.186	-8.058	5.066	1.00	41.42
MOTA	4477	0	ALA	575	52.392	-8.949	4.249	1.00	43.65
MOTA	4478	N	ARG	576	51.815	-8.294	6.319	1.00	42.56
ATOM	4480	CA	ARG	576	51.642	-9.646	6.824	1.00	42.51
ATOM	4481	CB	ARG	576	52.676	-9.910	7.920	1.00	40.14
MOTA	4482	CG	ARG	576	54.100	-9.896	7.377	1.00	40.32
MOTA	4483	CD	ARG	576	55.172	-9.836	8.460	1.00	40.78
MOTA	4484	NE	ARG	576	56.513	-9.783	7.874	1.00	42.13
MOTA	4486	CZ	ARG	576	56.975	-8.785	7.120	1.00	40.73
MOTA	4487	NH1	ARG	576	56.215	-7.732	6.851	1.00	39.21
ATOM	4490	NH2	ARG	576	58.201	-8.846	6.622	1.00	37.62
MOTA	4493	C	ARG	576	50.242	-9.931	7.326	1.00	44.48
MOTA	4494	0	ARG	576	50.028	-10.869	8.098	1.00	46.84
ATOM	4495	N	ARG	577	49.275	-9.146	6.866	1.00	46.26
ATOM	4497	CA	ARG	577	47.893	-9.344	7.292	1.00	46.89
ATOM	4498	CB	ARG	577	47.027	-8.170	6.845	1.00	46.16
MOTA	4499	CG	ARG	577	47.189	-6.939	7.696	1.00	44.93
MOTA	4500	CD	ARG	577	46.463	-5.766	7.080	1.00	44.60
MOTA	4501	NE	ARG	577	46.284	-4.683	8.039	1.00	45.05
MOTA	4503	CZ	ARG	577	45.612	-3.565	7.793	1.00	45.95
ATOM	4504	NH1	ARG	577	45.052	-3.372	6.606	1.00	47.39
MOTA	4507	NH2	ARG	577	45.466	-2.655	8.749	1.00	45.49
ATOM	4510	C	ARG	577	47.334	-10.649	6.740	1.00	46.60
ATOM	4511	0	ARG	577	47.478	-10.933	5.551	1.00	47.15
ATOM	4512	N	GLN	594	53.312	-14.007	7.967	1.00	63.97
MOTA	4514	CA	GLN	594	52.110	-14.068	8.799	1.00	63.06
MOTA	4515	CB	GLN	594	51.175	-15.183	8.319	1.00	64.16
MOTA	4516	С	GLN	594	52.501	-14.278	10.258	1.00	61.68
MOTA	4517	0	GLN	594	53.101	-15.292	10.619	1.00	60.95
MOTA	4518	N	LEU	595	52.140	-13.313	11.092	1.00	58.58
MOTA	4520	CA	LEU	595	52.470	-13.335	12.505	1.00	55.58
ATOM	4521	CB	LEU	595	52.619	-11.902	13.020	1.00	54.05
ATOM	4522	CG	LEU	595	53.570	-11.074	12.153	1.00	56.23
ATOM	4523	CD1	LEU	595	53.496	-9.609	12.524	1.00	58.84
MOTA	4524	CD2	LEU	595	54.977	-11.596	12.301	1.00	55.93
ATOM	4525	C	LEU	595	51.480	-14.093	13.372	1.00	53.77
MOTA	4526	0	LEU	595	50.276	-14.046	13.139	1.00	54.31
MOTA	4527	N	SER	596	52.012	-14.780	14.377	1.00	51.04
ATOM	4529	CA	SER	596	51.206	-15.541	15.316	1.00	48.97
ATOM	4530	CB	SER	596	52.004	-16.737	15.834	1.00	48.89
ATOM	4531	OG	SER	596	52.945	-16.345	16.820	1.00	48.59
ATOM	4533	C	SER	596	50.853	-14.641	16.488	1.00	47.56
ATOM	4534	0	SER	596	51.470	-13.590	16.676	1.00	46.71
ATOM	4535	N	SER	597	49.888	-15.070	17.292	1.00	47.11
ATOM	4537	CA	SER	597	49.462	-14.315	18.461	1.00	47.88
ATOM	4538	CB	SER	597	48.386	-15.084	19.229	1.00	50.66
MOTA	4539	OG	SER	597	47.574	-15.839	18.343	1.00	57.08
ATOM	4541	C	SER	597	50.666	-14.068	19.372	1.00	46.03
ATOM	4542	0	SER	597	50.735	-13.045	20.047	1.00	46.49
ATOM	4543	N	LYS	598	51.607	-15.007	19.399	1.00	46.08
ATOM	4545	CA	LYS	598	52.798	-14.844	20.229	1.00	46.33
ATOM	4546	CB	LYS	598	53.558	-16.163	20.384	1.00	46.67

59.841 -9.026 25.230 1.00 34.22

-9.300 26.109 1.00 36.64

				174		
ATOM 4	547 CG	LYS 5				
	548 CD		98 54.4.		224 21.623	3 0-
	549 CE	LYS 59	33.2	40 -17.5		47.01
T Constant	550 NZ	LYS 59	55.0	99 -17.7	97 23.026	- 55.65
*	54 C	LYS 59		91 -18.0		55.15
3 000		LYS 59	8 53.70			- 52.02
_		LYS 59	8 54.29			1.00 45.43
ATOM 45	E0 ~-	ASP 59	9 53.78			1.00 44.18
ATOM 45	CO ~-	ASP 59	9 54.59			1.00 44.16
3	ć0	ASP 599	9 54.52			1.00 43.46
3		ASP 599	55.28			1.00 44.83
		ASP 599	56.22			1.00 48.24
3000	_	ASP 599	54.95			1.00 52.90
3.770	- 4	ASP 599	54.120			1.00 51.43
ATOM 456		ASP 599				1.00 42.71
ATOM 456		EU 600			0 18.059	1.00 45.00
ATOM 456	7 CA I	EU 600	22.803			1 00
ATOM 456	n	EU 600	52.246		8 18.030	
ATOM 456	n	EU 600	50.747		2 17.747	_
ATOM 4570			50.332		16.281	_ <del>_</del>
ATOM 457]			48.814	-9.992		· · · · · · · · · · · · · · · · · · ·
ATOM 4572	. ~		50.974	-9.012		1.00 37.38
ATOM 4573			52.537	-9.452	10 40-	1.00 25.63
ATOM 4574			52.910	-8.294	10 62 -	1.00 34.58
ATOM 4576	~~ ~~		52.415	-10.348		1.00 33.18
ATOM 4577			52.692	-9.969		1.00 34.24
ATOM 4578			52.214	-11.036	20	1.00 35.80
ATOM 4579	VA		52.331	-10.483	24 2	1.00 37.50
ATOM 4580			50.766	-11.409		1.00 38.08
ATOM 4581	C VA		54.198	-9.741		1.00 40.77
ATOM 4582	O VA		54.634	-8.856		00 35.04
ATOM 4584	N SE		54.981	-10.531		.00 34.33
ATOM 4585	CA SEI		56.421	-10.421	21.262 1	.00 32.58
	CB SEI		57.045			.00 36.01
3770	OG SEF	602	58.453	-11.504	20.439 1	.00 38.43
N. Connection	C SEF	602	56.809	-11.387	20.419 1	.00 43.36
3.55	O SER	602	57.651	-9.038	20.800 1	.00 35.21
3.000	N CYS	603	56.183	-8.363	21.394 1.	.00 35.03
ATOM 4592	CA CYS		56.438	-8.614	19.707 1.	.00 34.15
ATOM 4593	CB CYS	603	55.543	-7.294	19.141 1.	00 34.04
ATOM 4594	SG CYS	603	55.653	~7.055 -	77 00-	00 33.45
ATOM 4595	C CYS	603	56.198	-5.423	17.229 0.	50 32.19 PRT1
ATOM 4596	O CYS	603	50.198	-6.211		00 32.79
ATOM 4597	N ALA	604	57.023	-5.316	20.362 1.	
ATOM 4599	CA ALA	604	55.088	-6.321		· <del>- •</del>
ATOM 4600	CB ALA	604	54.743	-5.358	21.965 1.0	
λ ποι	C ALA		53.321		22.481 1.0	
λ ΤΟΝ	O ALA	604	55.741		_	· · · · · · · · · · · · · · · · · · ·
አጥርኩ፣		604	56.050			
ATOM A		605	56.212			
ATTOM		605	57.189	_		· ·
7.000	CB TYR	605				
ATOM	CG TYR	605		_	24.737 1.0	
ATOM 4 de-	CD1 TYR	605	F0	_	25.690 1.0	0 32.51
ATOM 45-	CE1 TYR	605			7.053 1.0	0 33.50
3	D2 TYR	605	EO 044	-8.507 2	7.943 1.0	0 37.08
ATOM 4611 C	ידים מינים	<b>.</b>		-9.026 2	5 230 1 0	

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4611 CE2 TYR 605

60.896



ATOM	4612	CZ	TYR	605	60.746	-9.042	27.464	1.00	37.56
MOTA	4613	ОН	TYR	<b>60</b> 5	61.776	-9.342	28.336	1.00	38.08
MOTA	4615	С	TYR	605	58.480	-6.006	24.191	1.00	32.42
MOTA	4616	0	TYR	605	58.975	-5.203	24.991	1.00	33.34
MOTA	4617	N	GLN	606	58.997	-6.267	22.989	1.00	30.61
MOTA	4619	CA	GLN	606	60.218	-5.643	22.474	1.00	31.12
MOTA	4620	CB	GLN	606	60.499	-6.143	21.058	1.00	30.57
MOTA	4621	CG	GLN	606	61.044	-7.568	21.008	1.00	33.90
MOTA	4622	CD	GLN	606	61.240	-8.080	19.593	1.00	32.17
MOTA	4623	OE1	GLN	606	62.155	-7.652	18.883	1.00	32.55
ATOM	4624	NE2	GLN	606	60.374	-8.998	19.171	1.00	33.10
ATOM	4627	C	GLN	606	60.157	-4.114	22.487	1.00	31.69
MOTA	4628	0	GLN	606	61.111	-3.453	22.910	1.00	31.18
MOTA	4629	N	VAL	607	59.035	-3.564	22.020	1.00	29.50
MOTA	4631	CA	VAL	607	58.816	-2.122	22.000	1.00	27.54
ATOM	4632	CB	VAL	607	57.454	-1.751	21.306	1.00	26.79
ATOM	4633	CG1	VAL	607	57.131	-0.291	21.516	1.00	24.80
MOTA	4634	CG2	VAL	607	57.505	-2.050	19.815	1.00	22.95
MOTA	4635	C	LAV	607	58.827	-1.576	23.432	1.00	28.30
ATOM	4636	0	VAL	607	59.469	-0.548	23.705	1.00	28.32
MOTA	4637	N	ALA	608	58.110	-2.247	24.340	1.00	27.21
MOTA	4639	CA	ALA	608	58.061	-1.805	25.735	1.00	26.54
MOTA	4640	CB	ALA	608	57.070	-2.649	26.550	1.00	26.70
MOTA	4641	С	ALA	608	59.457	-1.850	26.368	1.00	25.97
MOTA	4642	0	ALA	608	59.802	-0.993	27.183	1.00	25.88
ATOM	4643	N	ARG	609	60.250	-2.848	25.994	1.00	26.02
MOTA	4645	CA	ARG	609	61.606	-2.977	26.512	1.00	30.44
ATOM	4646	CB	ARG	609	62.234	-4.285	26.058	1.00	34.09
ATOM	4647	CG	ARG	609	61.642	-5.516	26.682	1.00	39.24
MOTA	4648	CD	ARG	609	62.659	-6.615	26.615	1.00	42.75
ATOM	4649	NE	ARG	609	63.405	-6.704	27.860	1.00	45.52
ATOM	4651	CZ	ARG	609	64.525	-7.405	28.019	1.00	46.24
MOTA	4652	NH1	ARG	609	65.055	-8.079	27.001	1.00	41.48
ATOM	4655	NH2	ARG	609	65.079	-7.482	29.225	1.00	47.49
ATOM	4658	С	ARG	609	62.478	-1.829	26.015	1.00	34.20
MOTA	4659	0	ARG	609	63.265	-1.255	26.788	1.00	35.24
MOTA	4660	N	GLY	610	62.368	-1.528	24.717	1.00	33.25
MOTA	4662	CA	GLY	610	63.130	-0.439	24.138	1.00	29.57
MOTA	4663	С	GLY	610	62.802	0.814	24.908	1.00	29.31
ATOM	4664	0	GLY	610	63.695	1.543	25.335	1.00	27.46
MOTA	4665	N	MET	611	61.507	1.020	25.147	1.00	31.07
MOTA	4667	CA	MET	611	61.016	2.178	25.889	1.00	30.09
MOTA	4668	CB	MET	611	59.493	2.280	25.782	1.00	29.51
MOTA	4669	CG	MET	611	58.997	2.655	24.404	1.00	28.21
MOTA	4670	SD	MET	611	59.760	4.175	23.787	1.00	29.00
MOTA	4671	CE	MET	611	59.350	5.335	25.039	1.00	25.91
ATOM	4672	C	MET	611	61.439	2.189	27.361	1.00	30.47
ATOM	4673	0	MET	611	61.734	3.242	27.919	1.00	29.43
ATOM	4674	N	GLU	612	61.429	1.031	28.002	1.00	31.97
ATOM	4676	CA	GLU	612	61.836	0.947	29.402	1.00	35.34
ATOM	4677	CB	GLU	612	61.707	-0.490	29.904	1.00	36.17
MOTA	4678	CG	GLU	612	62.305	-0.729	31.278	1.00	34.87
ATOM	4679	CD	GLU	612	62.259	-2.185	31.705	1.00	32.68
MOTA	4680	OE1	GLU	612	62.641	-3.070	30.904	1.00	35.01

	ATOM	4603										
	ATOM	4681	OE2	GLU	612	61.8	848	٠.				
		4682	С	GLU	612	63.2	300	-2.4		.858	1.00	36.56
	ATOM	4683	0	GLU	612			1.4		490	1.00	35.26
		4684	N	TYR	613	63.6	77	2.16		417	1.00	
		4686	CA	TYR		64.0		1.04		491		31.21
	ATOM .	4687	CB		613	65.4		1.45		440	1.00	36.10
1		4688	CG	TYR	613	66.2	49	0.78			1.00	34.76
		1689		TYR	613	67.7		1.19			1.00	31.15
			CD1	TYR	613	68.6			-		1.00	34.28
		1690	CE1	TYR	613	69.9		0.65		207	1.00	36.50
	ma	691	CD2	TYR	613			1.03			1.00	38.20
	TOM 4	692	CE2	TYR	613	68.1	/9	2.13	5 26.3		1.00	32.99
		693	CZ	TYR	613	69.52		2.526	5 26.3		1.00	
A	TOM 4			TYR		70.39		1.968	3 27.3			33.32
A'			~		613	71.72		2.340			1.00	36.59
A:			_	I'YR	613	65.58		2.970			1.00	35.73
				ryr	613	66.23		3.643			.00	34.03
				LEU	614	64.91					00	35.26
			CA I	EU	614	64.94	_	3.503			.00	31.78
			CB I	ΈU	614	64.09		4.937			.00	29.50
	OM 47	'02 c	G [		614			5.297	25.7°			
		'03 C			514	64.564		1.742	24.42			28.26
AT	OM 47					63.564	! 5	.089	23.32			31.29
AT	OM 47	05 C	_		514	65.951	. 5	.282	24.07			28.09
AT	OM 47		_		14	64.489		.715			.00	29.52
ATO					14	65.108		.717	28.22		.00	32.49
ATO			_ 424		15	63.431			28.59		00 3	31.73
ATO				ЪА 6	15	62.906		.232	28.87			3.06
ATO			IA B	-	15	61.598		.870	30.07			5.16
			AI	A 6	15	63.942		.192	30.51			6.64
ATO		_	AL	_	15			.838	31.202	2 1.		5.36
ATO	-	.3 N	SE		16	64.065	6.	. 805	31.952			5.36
ATO		5 CA		_		64.690	4.	739	31.319		-	6.80
ATO					16	65.716		621	32.354			5.91
ATO	M 471					66.287		199	32.424			5.78
ATO	_					67.133		899				2.52
ATON	472		SE		6	66.832		623	31.324			.64
ATON			SEI	₹ 61	6	67.556			32.063	1.0		4.48
ATOM			LYS	61	7	66.971		048	32.967	1.0		.76
ATOM			LYS	61	7	67.973		980	30.790	1.0	_	. 74
	_		LYS	61	7			931	30.357	1.0		.44
ATOM	2 3	CG	LYS			68.540		520	28.998	1.0		. 94
ATOM		CD	LYS			69.330	5.2		29.041	1.0		
ATOM	4727	CE	LYS	617		70.539	5.4		29.933	1.00		. 64
ATOM	4728		LYS			71.252	4.0	91	30.139			. 45
ATOM		C				72.552	4.3		30.812	1.00		. 84
ATOM			LYS	617		67.376	8.3		30.012	1.00		
ATOM	4734	0	LYS	617		67.909	9.1		30.281	1.00	•	29
ATOM		N	LYS	618		6.245	8.5		29.598	1.00	33.	95
	4736	CA	LYS	618	6	55.569			0.952	1.00	34.	
ATOM	4737	CB	LYS	618		6.512	9.8		0.997	1.00	35.	44
ATOM	4738	CG	LYS	618			10.86	58 3	1.581	1.00	40.	
ATOM	4739	CD	LYS	618	-	7.192	10.44	<b>1</b> 6 3	2.877	1.00		
ATOM	4740	CE			6	6.234	10.36		4.037		48.	
ATOM	4741	NZ	LYS	618		6.962	9.93		5.310	1.00	55.	
ATOM	4745		LYS	618		6.070	10.03			1.00	61.	
ATOM		C	LYS	618		5.015	10.32		6.514	1.00	68.8	32
ATOM	4746	0	LYS	618		4.557			9.663	1.00	35.6	
	4747	N	CYS	619	6	5.006	11.46		9.569	1.00	36.4	
ATOM	4749	CA	CYS	619	<i>-</i>	1.525	9.47		3.647	1.00	34.2	
					0.		9.84			1.00	31.6	
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								_		31.3	. 7
				c10	61	5.279	9.033	26.263	1.00		
ATOM 4	750	CB	CYS	619		4.816	9.306	24.541	1.00		
ATOM 4	751	SG	CYS	619		3.004	9.701	27.149	1.00		24
	1752	С	CYS	619		2.418	8.649	27.388	1.00		
	1753	0	CYS	619		2.359	10.798	26.800	1.00		
	4754	N	ILE	620	6	0.935	10.822	26.542	1.00		
	4756	CA	ILE	620	6	0.935	12.040	27.193	1.00		26
	4757	CB	ILE	620	6	0.268	12.116	26.774	1.00	0 31.	
***	4758	CG2	ILE	620		8.799	11.957	28.712	1.0	0 29.	71
7.20	4759	CG1	ILE	620	6	50.392	13.236	29.396	1.0	0 27.	40
1120.	4760	CD1	ILE	620	•	60.016	10.961	25.023	1.0	0 31	. 86
111	4761	C	ILE	620		60.864	11.920	24.465	1.0		.70
111 0	4762	ō	ILE	620		61.384	9.986	24.366	1.0		.70
MOTA		N	HIS	621		60.249		22.906	1.0		.12
MOTA	4763	CA	HIS	621		60.133	9.973	22.430			.61
MOTA	4765	CB	HIS	623	L	59.708	8.578	20.961			.62
MOTA	4766		HIS		L	59.903	8.344	20.300			.49
MOTA	4767	CG				60.511	7.336				.08
MOTA	4768	CD2				59.373	9.168				.00
MOTA	4769					59.637	8.669				5.55
MOTA	4771					60.325	7.554				1.51
MOTA	4772		HI			59.194	11.026				5.79
MOTA	4774	_	HI			59.466	11.570				5.26
MOTA	4775					58.048	11.248			00 3	4.68
MOTA	4776		AR			57.068	12.239				3.43
MOTA	4778		AR		22	57.705	13.62				1.52
MOTA	4779				22	58.285	14.13	5 23.67			7.82
ATOM	478					58.781	15.56	3 23.5			8.82
ATOM	478	1 CD		_	22	59.216	16.05	0 24.8		_	30.41
MOTA		2 NE			22	60.362	15.71	5 25.40			31.15
MOTA		4 CZ		_	22	61.215	14.89	1 24.8		-	30.83
ATOM		5 NH			22	60.640	16.16	8 26.6		-	34.71
MOTA		8 NI			22	56.283	11.89	1 21.2			35.58
ATOM		91 C			22	55.289	12.54	4 20.9			34.90
ATOM		92 0			22	56.719		34, 20.4			34.90
MOTA		93 N	A		23	55.986		68 19.2			34.30
ATON		_	A A		523	56.443		12 17.9		-	36.76
ATO			в Р		523	55.535	_	18 16.		1.00	43.35
ATO			G I		623	55.980		31 15.0	524	1.00	47.64
ATO	_		D1 1		623	55.70				1.00	43.30
ATO:		99 C	D2 2	ASP	623	54.376 56.094	_			1.00	32.24
OTA		00 0	3	ASP	623		·		957	1.00	31.19
OTA		301 (		ASP	623	56.40	_		118	1.00	32.27
OTA	_		N	LEU	624	55.89			005	1.00	33.18
				LEU	624	55.96	-	118 21.	390	1.00	31.16
OTA				LEU	624	56.01	_	592 21.	452	1.00	32.74
)TA		-	CG	LEU	624	56.01	-		765	1.00	30.64
ATC		•••	CD1	LEU	624	57.25	•		904	1.00	34.51
TA		•••	CD2	LEU	624	55.97			.217	1.00	35.18
TA		_	CDZ	LEU	624	54.73		-	.612	1.00	35.72
	•••	809	0	LEU	624	53.58			.084	1.00	32.37
		810		ALA	625	54.9	-		.223	1.00	30.60
		811	N	ALA	625	53.9			.298	1.00	25.26
		1813	CA	ALA	625	53.4	47 6			1.00	29.87
	-	4814	CB	ALA	625	54.6	18 4		.427	1.00	32.01
A.	-	4815	С	ALA	625	~- ^		.978 16	3.378	1.00	
A.	rom ·	4816	0	MUM							

ATOM 4819 CA ALA 626 53.834 3.163 15.779 1.00 30.12 ATOM 4820 CB ALA 626 55.255 2.552 13.838 1.00 26.71 ATOM 4821 C ALA 626 55.255 2.552 13.838 1.00 26.29 ATOM 4822 O ALA 626 55.255 2.552 13.838 1.00 26.29 ATOM 4825 CA ARG 627 55.056 3.731 13.317 1.00 26.29 ATOM 4826 CC ARG 627 55.056 5.671 13.827 1.00 28.73 ATOM 4827 CB ARG 627 55.056 5.671 13.827 1.00 28.73 ATOM 4827 CB ARG 627 55.056 5.671 11.827 1.00 29.83 ATOM 4827 CB ARG 627 55.056 5.671 11.827 1.00 29.83 ATOM 4828 CD ARG 627 55.056 6.659 12.972 1.00 31.84 ATOM 4829 NE ARG 627 54.435 8.032 12.485 1.00 38.59 ATOM 4829 NE ARG 627 55.2745 8.879 14.064 1.00 39.55 ATOM 4831 C 2 ARG 627 55.2745 8.879 14.064 1.00 39.55 ATOM 4839 NH1 ARG 627 55.056 4.559 12.274 1.00 29.83 ATOM 4839 NH2 ARG 627 55.1822 8.094 13.525 1.00 31.84 ATOM 4839 NH2 ARG 627 57.151 4.632 12.676 1.00 30.79 ATOM 4839 C ARG 627 55.056 4.659 12.00 30.079 ATOM 4840 N ASN 628 57.347 9.604 15.127 1.00 31.84 ATOM 4840 N ASN 628 57.347 9.604 15.127 1.00 31.84 ATOM 4840 N ASN 628 57.347 1.632 11.838 1.00 30.16 ATOM 4841 CG ASN 628 58.661 5.109 14.550 1.00 30.16 ATOM 4843 CB ASN 628 58.587 5.159 14.652 11.985 1.00 33.45 ATOM 4846 ND2 ASN 628 58.893 7.796 13.782 1.00 33.45 ATOM 4846 ND2 ASN 628 58.893 7.796 13.782 1.00 33.45 ATOM 4851 C ASN 628 59.352 3.919 15.169 1.00 28.50 ATOM 4851 C ASN 628 59.352 3.919 15.169 1.00 28.10 ATOM 4858 C C VAL 629 59.887 1.751 14.868 1.00 33.45 ATOM 4856 C C VAL 629 59.980 1.266 17.265 1.00 28.50 ATOM 4857 C VAL 629 59.980 1.266 17.265 1.00 29.48 ATOM 4865 C C ARG 627 57.551 6.20 1.00 29.48 ATOM 4866 C C ARG 627 59.400 1.00 1.00 29.98 ATOM 4867 C VAL 629 59.980 1.266 17.265 1.00 29.62 ATOM 4868 C C VAL 629 59.887 1.00 1.00 29.98 ATOM 4867 C VAL 629 59.887 1.00 1.00 29.98 ATOM 4868 C C VAL 629 59.887 1.00 1.00 29.98 ATOM 4867 C VAL 629 59.980 1.266 1.00 31.00 29.99 ATOM 4868 C C VAL 631 63.062 1.00 1.00 29.98 ATOM 4867 C VAL 631 63.062 1.00 1.00 31.80 ATOM 4868 C C VAL 631 63.062 1.00 1.00 31.80 ATOM 4868 C C VAL 631 63.062 1.00 1.00 31.80 ATOM 4868 C C VAL 631 63.062 1.0		ATOM	4817						_				
ATOM 4821 C					ALA	626	53.	834	,				
ATOM 4821 C ALA 626 51.231 1.159 14.441 1.00 29.62 ATOM 4822 O ALA 626 51.231 1.159 14.441 1.00 27.11 ATOM 4823 N ARG 627 55.255 13.838 1.00 27.11 ATOM 4825 CA ARG 627 55.056 3.730 13.434 1.00 26.29 ATOM 4826 CB ARG 627 55.056 4.352 12.244 1.00 28.73 ATOM 4828 CD ARG 627 55.056 5.671 11.871 13.471 1.00 26.74 ATOM 4828 CD ARG 627 55.056 5.671 12.271 1.00 28.73 ATOM 4829 N ARG 627 55.056 5.671 12.271 1.00 31.84 ATOM 4821 CD ARG 627 54.455 8.032 12.485 1.00 31.84 ATOM 4828 CD ARG 627 54.455 8.032 12.485 1.00 31.85 ATOM 4831 CZ ARG 627 52.745 8.879 11.590 1.00 31.85 ATOM 4831 N ARG 627 52.745 8.879 11.590 1.00 31.596 ATOM 4835 NH2 ARG 627 52.447 9.604 13.525 1.00 31.596 ATOM 4839 O ARG 627 55.151 4.686 11.838 1.00 30.76 ATOM 4839 C ARG 627 55.347 4.687 11.838 1.00 30.16 ATOM 4840 N ASN 628 58.661 5.109 14.550 10.0 30.31 ATOM 4844 CA ASN 628 57.347 4.687 11.838 1.00 30.16 ATOM 4844 CA ASN 628 58.661 5.109 14.550 1.00 30.31 ATOM 4844 CA ASN 628 58.661 5.109 14.550 1.00 30.31 ATOM 4844 CA ASN 628 58.869 7.571 14.868 1.00 30.16 ATOM 4844 CA ASN 628 58.869 7.571 14.868 1.00 30.16 ATOM 4844 CA ASN 628 58.869 7.571 14.868 1.00 30.16 ATOM 4844 ND ASN 628 58.869 7.571 14.868 1.00 30.16 ATOM 4846 ND ASN 628 58.869 7.571 14.868 1.00 31.41 ATOM 4846 ND ASN 628 58.869 7.571 14.868 1.00 31.41 ATOM 4855 CG ASN 628 59.352 8.499 15.460 1.00 28.50 ATOM 4856 C VAL 629 59.455 0.577 15.983 1.00 28.30 ATOM 4856 C C VAL 629 59.455 0.577 15.983 1.00 28.30 ATOM 4856 C C VAL 629 59.456 1.220 1.00 30.51 ATOM 4856 C C VAL 629 59.456 1.220 1.00 30.51 ATOM 4857 C VAL 629 59.457 0.577 15.983 1.00 28.30 ATOM 4858 C C VAL 629 59.454 1.462 15.255 1.00 33.45 ATOM 4857 C VAL 629 59.454 1.462 15.255 1.00 29.48 ATOM 4857 C VAL 629 59.454 1.462 15.255 1.00 29.48 ATOM 4858 C C VAL 631 62.290 1.140 0.616 13.043 1.00 27.79 ATOM 4857 C VAL 629 59.456 1.140 0.616 13.043 1.00 29.79 ATOM 4867 C C VAL 631 62.290 1.140 0.616 13.043 1.00 29.79 ATOM 4867 C C VAL 631 62.290 1.140 0.616 13.043 1.00 29.94 ATOM 4879 C B VAL 631 62.274 3.863 1.128 1.00 32.37 ATOM 4879					ALA	626							30 12
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ATOM 4827 CG ARG 627 55.056 6.675 11.827 1.00 29.62 ATOM 4828 CD ARG 627 54.894 6.659 12.972 1.00 31.84 ATOM 4829 NE ARG 627 53.987 8.878 13.590 1.00 38.59 ATOM 4831 CZ ARG 627 51.822 8.094 13.525 1.00 38.59 ATOM 4838 C ARG 627 57.151 4.632 15.251 1.00 39.55 ATOM 4838 C ARG 627 57.151 4.632 12.676 1.00 30.16 ATOM 4840 N ASN 628 57.347 9.604 15.127 1.00 30.16 ATOM 4840 N ASN 628 58.587 6.257 11.838 1.00 30.16 ATOM 4843 CG ASN 628 58.661 5.09 14.550 1.00 30.31 ATOM 4846 ND2 ASN 628 58.893 7.796 13.782 1.00 30.31 ATOM 4848 CG ASN 628 58.893 7.796 13.782 1.00 30.31 ATOM 4846 ND2 ASN 628 58.893 7.796 13.782 1.00 31.45 ATOM 4855 CD ASN 628 59.352 3.999 15.640 31.45 ATOM 4855 CB VAL 629 59.484 1.482 11.800 22.538 ATOM 4854 CB VAL 629 59.484 1.482 11.00 22.538 ATOM 4855 CB VAL 629 59.118 0.577 15.993 1.00 28.50 ATOM 4856 CB VAL 629 59.118 0.577 15.993 1.00 28.50 ATOM 4856 CB VAL 629 59.911 0.616 13.949 1.00 28.53 ATOM 4856 CB VAL 629 59.912 0.573 14.803 1.00 27.94 ATOM 4856 CB VAL 629 59.925 0.810 13.949 1.00 28.50 ATOM 4856 CB VAL 629 59.918 0.577 15.993 1.00 28.00 ATOM 4866 C LEU 630 61.220 0.542 13.823 1.00 27.95 ATOM 4867 C VAL 629 59.918 0.616 13.949 1.00 28.00 ATOM 4866 C LEU 630 61.200 0.542 13.823 1.00 27.95 ATOM 4867 C VAL 629 59.925 0.810 13.949 1.00 28.69 ATOM 4866 C LEU 630 61.693 2.599 0.659 12.142 1.00 23.07 ATOM 4867 C VAL 631 63.629 59.114 0.616 13.949 1.00 28.69 ATOM 4868 N VAL 631 63.629 59.114 0.616 13.949 1.00 28.69 ATOM 4868 C VAL 631 63.06 62.290 1.141 0.66 13.949 1.00 28.983 ATOM 4868 C VAL 631 63.06 62.290 1.141 0.66 13.949 1.00 28.983 ATOM 4868 C VAL 631 63.06 62.390 1.244 12.899 1.00 29.983 ATOM 4868 C C RAM 631 63.379 4.242 11.196 1.00 33.03 ATOM 4868 C C RAM 632 66.659 -5.665 12.148 1.00 33.03 ATOM 4870 CA VAL 631 63.379 4.242 11.196 1.00 33.57 ATOM 4871 CB VAL 631 63.379 4.242 11.196 1.00 33.57 ATOM 4872 CG VAL 631 63.379 4.242 11.196 1.00 33.57 ATOM 4878 CA VAL 631 63.379 4.242 11.196 1.00 33.57 ATOM 4878 CA VAL 631 63.379 4.242 11.196 1.00 33.57 ATOM 4878 CA VAL 631 63.379 4.242 11.196 1.		ATOM	4826				55.	706			10.01/		26.74
ATOM 4828 CD ARG 627 54.894 6.659 12.972 1.00 32.52 ATOM 4829 NE ARG 627 53.987 8.032 12.485 1.00 38.54 ATOM 4831 NEL ARG 627 53.987 8.032 12.485 1.00 38.54 ATOM 4832 NH1 ARG 627 52.745 8.899 14.064 1.00 38.59 ATOM 4838 NH2 ARG 627 52.745 8.899 14.064 1.00 39.55 ATOM 4838 NH2 ARG 627 52.447 9.604 15.127 1.00 15.96 ATOM 4839 O ARG 627 52.447 9.604 15.127 1.00 15.96 ATOM 4839 O ARG 627 57.151 4.632 12.676 1.00 30.79 ATOM 4840 N ASN 628 57.347 4.622 12.676 1.00 30.79 ATOM 4843 CB ASN 628 58.587 6.257 15.5549 1.00 30.16 ATOM 4844 CG ASN 628 58.587 6.257 15.5549 1.00 28.50 ATOM 4845 ODI ASN 628 58.889 7.571 14.868 1.00 31.41 ATOM 4848 OND ASN 628 58.889 7.571 14.868 1.00 31.41 ATOM 4851 N VAL 629 59.352 3.919 15.169 1.00 28.50 ATOM 4851 N VAL 629 59.484 1.00 27.79 ATOM 4855 CG VAL 629 59.952 0.810 13.949 1.00 28.63 ATOM 4856 CG VAL 629 59.944 1.00 27.79 ATOM 4857 C VAL 629 59.118 0.577 15.983 1.00 23.07 ATOM 4858 C C VAL 629 59.925 0.810 13.949 1.00 28.69 ATOM 4859 N LEU 630 61.220 0.542 13.823 1.00 23.07 ATOM 4864 CD LEU 630 61.220 0.542 13.823 1.00 29.54 ATOM 4865 CD LEU 630 62.299 0.659 11.579 1.00 29.64 ATOM 4866 C C VAL 629 59.144 0.00 27.79 ATOM 4867 C LEU 630 61.220 0.542 13.823 1.00 29.54 ATOM 4868 N LEU 630 61.220 0.542 13.823 1.00 29.54 ATOM 4867 C VAL 629 59.144 0.061 13.043 1.00 27.07 ATOM 4868 N LEU 630 61.249 0.549 11.866 1.00 30.17 ATOM 4868 N LEU 630 62.299 0.659 12.669 1.00 29.14 ATOM 4868 N VAL 631 61.966 2.230 1.1541 1.00 29.54 ATOM 4868 N VAL 631 61.966 2.230 1.1541 1.00 29.53 ATOM 4867 C VAL 631 60.992 1.00 0.542 13.823 1.00 29.54 ATOM 4868 N VAL 631 61.966 2.376 11.866 1.00 30.17 ATOM 4868 N VAL 631 61.966 2.376 11.866 1.00 30.17 ATOM 4870 C R VAL 631 63.379 4.242 11.966 1.00 29.39 ATOM 4868 N VAL 631 61.966 2.376 11.866 1.00 31.03 ATOM 4870 C R VAL 631 63.379 4.242 11.966 1.00 25.38 ATOM 4870 C R VAL 631 60.992 4.666 59 1.543 11.00 29.53 ATOM 4882 CG2 THR 632 66.286 -5.664 1.00 33.13 ATOM 4882 CG2 THR 632 66.286 -7.74 13.000 10.0 34.88 ATOM 4882 CG2 THR 632 66.286 -7.74 13.000 10.0 37.63		ATOM					55.0	<b>95</b> 6			12.244		
ATOM 4829 NE ARG 627 53.987 8.032 12.485 1.00 38.54 ATOM 4831 CZ ARG 627 53.987 8.878 13.590 1.00 38.59 ATOM 4835 NH1 ARG 627 52.745 8.879 14.064 1.00 39.55 ATOM 4835 NH2 ARG 627 52.447 9.604 15.127 1.00 41.05 ATOM 4836 C ARG 627 57.151 9.604 15.127 1.00 41.05 ATOM 4840 N ASN 628 57.347 4.632 12.676 1.00 30.16 ATOM 4843 CR ASN 628 57.347 4.632 12.676 1.00 30.16 ATOM 4843 CR ASN 628 57.347 4.822 13.985 1.00 30.16 ATOM 4844 CG ASN 628 58.661 5.109 14.550 1.00 28.50 ATOM 4844 CG ASN 628 58.887 6.257 15.549 1.00 27.84 ATOM 4845 OD1 ASN 628 58.893 7.796 13.782 1.00 33.45 ATOM 4846 ND2 ASN 628 58.893 7.796 13.782 1.00 33.45 ATOM 4850 C ASN 628 59.352 8.429 15.460 1.00 28.53 ATOM 4851 N VAL 629 59.484 1.482 15.253 1.00 33.45 ATOM 4855 CG1 VAL 629 59.484 1.482 15.253 1.00 22.88 ATOM 4856 CG2 VAL 629 59.118 -0.753 16.284 1.00 22.48 ATOM 4856 CG2 VAL 629 59.118 -0.753 16.284 1.00 22.48 ATOM 4856 CG2 VAL 629 59.118 -0.753 16.284 1.00 22.48 ATOM 4856 CG2 VAL 629 59.118 -0.753 16.284 1.00 22.48 ATOM 4856 CG2 VAL 629 59.118 -0.753 16.284 1.00 22.48 ATOM 4856 CG2 VAL 629 59.118 -0.753 16.284 1.00 22.48 ATOM 4856 CG2 VAL 629 59.118 -0.753 16.284 1.00 22.48 ATOM 4856 CG2 VAL 629 59.118 -0.753 16.284 1.00 22.48 ATOM 4856 CG2 VAL 629 59.118 -0.753 16.284 1.00 22.48 ATOM 4856 CG2 VAL 629 59.118 -0.753 16.284 1.00 22.48 ATOM 4856 CG2 VAL 629 59.118 -0.753 16.284 1.00 22.48 ATOM 4856 CG2 VAL 629 59.118 -0.753 16.284 1.00 22.48 ATOM 4856 CG2 VAL 630 61.693 2.543 11.086 1.00 32.59 ATOM 4860 C LEU 630 62.290 -1.910 14.062 1.00 30.17 ATOM 4860 C LEU 630 62.290 -1.910 14.062 1.00 32.59 ATOM 4870 CA VAL 631 61.966 -2.376 11.866 1.00 32.39 ATOM 4871 CB VAL 631 61.966 -2.376 11.866 1.00 32.39 ATOM 4873 CG2 VAL 631 62.474 -3.813 12.022 1.00 33.03 ATOM 4873 CG2 VAL 631 62.744 -3.813 12.022 1.00 33.03 ATOM 4874 C VAL 631 63.379 -4.242 11.196 1.00 22.39 ATOM 4878 C CG2 THR 632 66.550 -5.565 1.910 1.00 30.766 ATOM 4884 CD THR 632 66.550 -7.566 1.00 33.70 ATOM 4884 C THR 632 66.550 -7.568 11.168 1.00 33.720	į	ATOM				627	54.8	394			11.827	1.00	
ATOM 4832 NH1 ARG 627 53.987 8.878 13.590 1.00 38.59 ATOM 4832 NH1 ARG 627 52.745 8.879 14.064 1.00 39.55 ATOM 4838 NH2 ARG 627 52.447 9.604 13.525 1.00 35.96 ATOM 4839 O ARG 627 57.151 4.632 12.676 1.00 30.79 ATOM 4840 N ASN 628 57.347 4.822 13.985 1.00 30.79 ATOM 4841 CB ASN 628 58.661 5.109 14.550 1.00 30.31 ATOM 4842 CA ASN 628 58.661 5.109 14.550 1.00 30.31 ATOM 4845 CB ASN 628 58.587 6.257 15.549 1.00 30.31 ATOM 4846 ND2 ASN 628 58.893 7.571 14.868 1.00 31.41 ATOM 4849 C ASN 628 58.893 7.571 14.868 1.00 31.41 ATOM 4840 ND2 ASN 628 58.893 7.571 14.868 1.00 31.41 ATOM 4840 ND2 ASN 628 59.352 3.919 15.160 1.00 28.50 ATOM 4840 ND2 ASN 628 59.352 3.919 15.160 1.00 28.53 ATOM 4851 N VAL 629 58.887 2.733 14.803 1.00 27.79 ATOM 4854 CB VAL 629 59.484 1.482 15.253 1.00 28.30 ATOM 4855 CG1 VAL 629 59.484 1.482 15.253 1.00 28.30 ATOM 4856 CG2 VAL 629 59.484 1.482 15.253 1.00 22.48 ATOM 4858 O VAL 629 59.925 0.810 1.246 17.265 1.00 23.07 ATOM 4858 C VAL 629 59.91 1.246 17.265 1.00 23.07 ATOM 4858 C VAL 629 59.91 1.246 17.265 1.00 23.07 ATOM 4858 C VAL 629 59.91 1.246 17.265 1.00 23.07 ATOM 4858 C C VAL 629 59.91 1.246 17.265 1.00 23.07 ATOM 4858 C C VAL 629 59.91 1.246 17.265 1.00 23.07 ATOM 4866 C LEU 630 61.749 -0.081 12.616 1.00 29.64 ATOM 4866 C LEU 630 62.831 1.366 1.00 29.54 ATOM 4866 C LEU 630 62.831 1.366 1.00 29.54 ATOM 4866 C LEU 630 62.831 1.289 1.00 29.54 ATOM 4866 C LEU 630 62.831 1.586 1.00 29.14 ATOM 4867 C VAL 631 63.508 -1.541 12.899 1.00 33.05 ATOM 4868 N VAL 631 63.508 -3.865 11.866 1.00 33.03 ATOM 4870 CA VAL 631 63.508 -3.865 11.820 1.00 29.39 ATOM 4871 CB VAL 631 63.508 -3.865 11.180 1.00 29.39 ATOM 4872 CG1 VAL 631 63.508 -3.865 11.180 1.00 29.39 ATOM 4873 CG2 VAL 631 63.508 -3.865 11.180 1.00 32.37 ATOM 4873 CG2 VAL 631 63.508 -3.865 11.180 1.00 33.57 ATOM 4874 C VAL 631 63.508 -3.865 11.180 1.00 33.57 ATOM 4876 N THR 632 66.529 -5.685 11.180 1.00 33.70 ATOM 4880 C THR 632 66.629 -5.685 11.180 1.00 33.70 ATOM 4880 C THR 632 66.629 -7.568 11.180 1.00 33.70 ATOM 4884 C THR 632 66.295 -7.568 11.1		7.000			ARG	627	54.4	35				1.00	31 84
ATOM 4835 NH1 ARG 627 51.822 8.879 14.064 1.00 38.59 ATOM 4835 NH1 ARG 627 51.822 8.094 13.550 1.00 35.96 ATOM 4838 C ARG 627 52.447 9.604 15.127 1.00 41.05 ATOM 4840 N ASN 628 57.347 4.632 12.676 1.00 30.16 ATOM 4842 CA ASN 628 58.661 4.632 12.676 1.00 30.16 ATOM 4843 CB ASN 628 58.661 1.838 1.00 30.16 ATOM 4844 CG ASN 628 58.661 5.109 14.550 1.00 30.31 ATOM 4845 ODI ASN 628 58.897 7.571 14.868 1.00 30.31 ATOM 4846 ND2 ASN 628 58.893 7.796 13.782 1.00 27.84 ATOM 4846 ND2 ASN 628 59.352 3.919 15.460 1.00 28.53 ATOM 4851 N VAL 629 58.887 7.796 13.782 1.00 28.50 ATOM 4851 N VAL 629 59.484 1.482 15.169 1.00 28.50 ATOM 4855 CG VAL 629 59.484 1.482 15.253 1.00 28.30 ATOM 4855 CG VAL 629 59.18 -0.573 16.284 1.00 28.30 ATOM 4856 CG VAL 629 59.18 -0.573 16.284 1.00 22.307 ATOM 4857 C VAL 629 59.911 -0.5753 16.284 1.00 22.307 ATOM 4858 O VAL 629 59.911 -0.5753 16.284 1.00 22.307 ATOM 4856 CG VAL 629 59.911 -0.5753 16.284 1.00 22.307 ATOM 4857 C VAL 629 59.925 0.810 13.949 1.00 22.307 ATOM 4858 O VAL 629 59.911 -0.5753 16.284 1.00 22.307 ATOM 4857 C VAL 629 59.911 -0.5753 16.284 1.00 22.307 ATOM 4858 O VAL 629 59.911 -0.5753 16.284 1.00 22.307 ATOM 4859 N LEU 630 61.200 0.552 13.823 1.00 27.07 ATOM 4866 CD LEU 630 61.693 2.543 11.806 1.00 29.62 ATOM 4866 CD LEU 630 62.831 2.100 0.559 1.00 29.62 ATOM 4867 CD LEU 630 62.831 2.100 0.591 1.242 1.00 29.62 ATOM 4868 N VAL 631 61.693 2.543 11.806 1.00 32.59 ATOM 4870 CA VAL 631 61.966 -2.376 11.806 1.00 32.59 ATOM 4870 CA VAL 631 61.966 -2.376 11.806 1.00 32.59 ATOM 4871 CB VAL 631 61.966 -2.376 11.806 1.00 32.59 ATOM 4873 CG VAL 631 61.966 -2.376 11.800 1.00 32.59 ATOM 4870 CA VAL 631 63.508 -3.865 10.024 1.00 33.03 ATOM 4871 CB VAL 631 63.508 -3.865 10.024 1.00 32.37 ATOM 4872 CG VAL 631 63.508 -3.865 10.024 1.00 33.57 ATOM 4873 CG VAL 631 63.508 -3.865 10.024 1.00 32.37 ATOM 4874 C VAL 631 63.508 -3.865 10.024 1.00 33.57 ATOM 4879 CB THR 632 66.289 -5.685 12.1448 1.00 33.70 ATOM 4883 C THR 632 66.289 -7.161 1.00 4.99 1.00 33.70					ARG	627					12.485		38 54
ATOM 4832 NH1 ARG 627 51.822 8.094 13.525 1.00 39.55 96 ATOM 4838 C ARG 627 52.447 9.604 15.127 1.00 41.05 96 ATOM 4839 O ARG 627 55.151 4.632 12.676 1.00 30.79 ATOM 4830 N ASN 628 57.347 4.822 13.985 1.00 30.16 ATOM 4842 CA ASN 628 58.661 5.109 14.550 1.00 30.31 ATOM 4844 CG ASN 628 58.661 5.109 14.550 1.00 30.31 ATOM 4845 OD1 ASN 628 58.587 6.257 15.549 1.00 30.31 ATOM 4845 OD1 ASN 628 58.893 7.571 14.868 1.00 31.41 ATOM 4845 OD1 ASN 628 59.352 3.919 15.169 1.00 28.50 ATOM 4851 N VAL 629 59.887 2.733 14.803 1.00 28.53 ATOM 4853 CA VAL 629 59.484 1.482 15.253 1.00 28.70 ATOM 4855 CGI VAL 629 59.484 1.482 15.253 1.00 28.70 ATOM 4856 CG2 VAL 629 59.484 1.482 15.253 1.00 23.07 ATOM 4856 CG2 VAL 629 59.915 0.801 13.949 1.00 23.07 ATOM 4864 CB VAL 629 59.915 0.801 13.949 1.00 23.07 ATOM 4864 CB VAL 629 59.915 0.801 13.949 1.00 23.07 ATOM 4865 CB LEU 630 61.749 -0.081 12.616 1.00 30.17 ATOM 4866 CB LEU 630 61.749 -0.081 12.616 1.00 30.17 ATOM 4866 CB LEU 630 61.749 -0.081 12.616 1.00 29.54 ATOM 4866 CB LEU 630 62.891 0.554 11.589 1.00 29.54 ATOM 4867 CD LEU 630 62.891 0.554 11.580 1.00 29.54 ATOM 4866 CB LEU 630 61.749 -0.081 12.616 1.00 30.17 ATOM 4866 CB LEU 630 61.749 -0.081 12.616 1.00 30.17 ATOM 4866 CB LEU 630 62.891 0.554 11.589 1.00 29.62 ATOM 4866 CB LEU 630 62.891 0.554 11.589 1.00 29.54 ATOM 4866 CB LEU 630 62.891 1.596 1.599 1.00 29.54 ATOM 4866 CB LEU 630 62.891 1.596 1.599 1.00 29.54 ATOM 4866 CB LEU 630 62.891 1.596 1.599 1.00 29.54 ATOM 4866 CB LEU 630 62.891 1.596 1.599 1.00 29.30 ATOM 4866 CB LEU 630 62.891 1.596 1.599 1.00 29.39 ATOM 4870 CA VAL 631 61.017 6.607 11.980 1.00 29.39 ATOM 4870 CA VAL 631 61.017 6.607 11.980 1.00 29.39 ATOM 4870 CA VAL 631 61.017 6.607 11.980 1.00 29.39 ATOM 4870 CA VAL 631 61.017 6.607 11.980 1.00 29.39 ATOM 4870 CA VAL 631 61.017 6.607 11.980 1.00 29.39 ATOM 4870 CA VAL 631 61.017 6.607 11.980 1.00 29.39 ATOM 4870 CA VAL 631 61.017 6.607 11.980 1.00 29.39 ATOM 4870 CA VAL 631 61.017 6.607 11.980 1.00 29.39 ATOM 4870 CA VAL 631 61.017 6.628 6.629 7.5685 11.180 1.00 29				CZ	ARG		50.7	4.5			3.590		
ATOM 4835 NH2 ARG 627 52.447 9.604 15.127 1.00 35.96 ATOM 4839 0 ARG 627 57.151 4.632 12.676 1.00 30.79 ATOM 4839 0 ARG 627 57.151 4.632 12.676 1.00 30.79 ATOM 4840 N ASN 628 57.347 4.822 13.985 1.00 30.31 ATOM 4841 CG ASN 628 58.587 6.257 15.549 1.00 30.31 ATOM 4844 CG ASN 628 58.369 7.571 14.868 1.00 30.16 ATOM 4846 ND2 ASN 628 58.369 7.571 14.868 1.00 31.41 ATOM 4846 ND2 ASN 628 59.352 3.919 15.460 1.00 28.50 ATOM 4851 N VAL 629 59.352 3.919 15.169 1.00 28.10 ATOM 4851 N VAL 629 59.484 1.482 15.253 1.00 28.10 ATOM 4854 CB VAL 629 59.484 1.482 15.253 1.00 28.10 ATOM 4855 CG1 VAL 629 59.484 1.482 15.253 1.00 28.30 ATOM 4856 CG2 VAL 629 59.118 0.753 16.284 1.00 27.79 ATOM 4857 C VAL 629 59.118 0.753 16.284 1.00 23.07 ATOM 4856 CG2 VAL 629 59.118 0.753 16.284 1.00 22.488 ATOM 4857 C VAL 629 59.114 0.616 13.043 1.00 27.07 ATOM 4856 CG LEU 630 61.749 0.061 13.949 1.00 28.69 ATOM 4866 C LEU 630 62.831 2.180 12.616 1.00 29.62 ATOM 4866 C LEU 630 62.831 2.180 12.616 1.00 29.62 ATOM 4866 C LEU 630 62.831 2.180 12.035 1.00 29.54 ATOM 4866 C LEU 630 62.290 1.246 12.055 10.00 29.48 ATOM 4867 O LEU 630 62.290 -1.541 12.899 1.00 29.62 ATOM 4868 N VAL 631 63.062 -1.541 12.899 1.00 29.62 ATOM 4872 CG1 VAL 631 63.079 -4.242 11.196 1.00 29.39 ATOM 4873 CG2 VAL 631 63.079 -4.242 11.196 1.00 25.38 ATOM 4870 CA VAL 631 63.379 -4.242 11.196 1.00 25.38 ATOM 4870 CA VAL 631 63.379 -4.242 11.196 1.00 25.38 ATOM 4870 CA VAL 631 63.379 -4.242 11.196 1.00 25.38 ATOM 4870 CN VAL 631 63.379 -4.242 11.196 1.00 25.38 ATOM 4870 CA VAL 631 63.379 -4.242 11.196 1.00 25.38 ATOM 4870 CA VAL 631 63.379 -4.242 11.196 1.00 25.38 ATOM 4870 CA VAL 631 63.596 -4.285 -4.987 11.820 1.00 33.11 ATOM 4870 CA VAL 631 63.692 -4.665 11.582 1.00 33.131 ATOM 4870 CA VAL 631 63.596 -5.685 12.148 1.00 33.131 ATOM 4870 CA VAL 631 63.079 -4.242 11.196 1.00 32.37 ATOM 4870 CA VAL 631 63.079 -4.242 11.196 1.00 32.37 ATOM 4870 CA VAL 631 63.090 -4.242 11.196 1.00 33.131 ATOM 4870 CA VAL 631 63.090 -4.242 11.196 1.00 33.131 ATOM 4880 CG1 THR 632 66.659 -7.547 13.000 10		m		NH1	ARG		52.7	45	8.8				
ATOM 4838 C ARG 627 57.151 4.632 12.676 1.00 30.79 ATOM 4840 N ASN 628 57.347 4.822 13.985 1.00 30.16 ATOM 4840 C ASN 628 57.347 4.822 13.985 1.00 30.16 ATOM 4841 CB ASN 628 58.587 6.257 15.549 14.550 1.00 28.50 ATOM 4845 OD1 ASN 628 58.587 6.257 15.549 14.550 1.00 28.50 ATOM 4846 ND2 ASN 628 58.893 7.796 13.782 1.00 33.45 ATOM 4845 OD1 ASN 628 57.551 8.429 15.460 1.00 28.53 ATOM 4850 O ASN 628 57.551 8.429 15.460 1.00 28.53 ATOM 4851 N VAL 629 58.887 4.076 16.021 1.00 28.53 ATOM 4854 CB VAL 629 59.484 1.482 15.253 1.00 28.30 ATOM 4855 CG1 VAL 629 59.484 1.482 15.253 1.00 28.30 ATOM 4856 CG2 VAL 629 59.118 -0.753 16.284 1.00 23.07 ATOM 4857 C VAL 629 59.915 0.577 15.983 1.00 25.38 ATOM 4859 N LEU 630 61.220 0.542 13.823 1.00 22.48 ATOM 4850 CG LEU 630 61.220 0.542 13.823 1.00 29.54 ATOM 4858 CG LEU 630 62.999 0.659 12.42 1.00 29.62 ATOM 4856 CG LEU 630 62.999 0.659 1.242 1.00 29.62 ATOM 4857 C VAL 629 59.114 0.616 13.043 1.00 27.07 ATOM 4863 CG LEU 630 62.999 0.659 1.242 1.00 29.62 ATOM 4866 C LEU 630 62.999 0.659 1.242 1.00 29.62 ATOM 4867 C LEU 630 62.999 0.659 1.242 1.00 29.62 ATOM 4868 N VAL 631 61.966 -2.376 11.866 1.00 30.17 ATOM 4866 C LEU 630 62.290 -1.541 12.899 1.00 30.50 ATOM 4867 C VAL 631 63.309 -1.541 12.899 1.00 30.50 ATOM 4868 N VAL 631 63.309 -1.541 12.899 1.00 30.50 ATOM 4868 N VAL 631 60.902 -4.605 11.582 1.00 29.88 ATOM 4870 CA VAL 631 63.309 -4.605 11.582 1.00 29.88 ATOM 4870 CA VAL 631 63.309 -4.242 11.196 1.00 33.303 ATOM 4870 CA VAL 631 63.309 -4.242 11.196 1.00 33.57 ATOM 4876 N THR 632 66.592 -4.987 11.820 1.00 33.57 ATOM 4878 CG THR 632 66.592 -5.685 12.148 1.00 33.11 ATOM 4878 CG THR 632 66.592 -5.685 12.148 1.00 33.11 ATOM 4884 O THR 632 66.592 -7.347 10.439 1.00 37.20			835	NH2			51.8	22	8.0				
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33.78	SSSDIE	1 45						-/.16	3	9.600			
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MOTA	4887	CA	GLU	633	66.182	-8.379	8.794	1.00	43.30
MOTA	4888	CB	GLU	633	67.437	-8.590	7.933	1.00	46.66
ATOM	4889	CG	GLU	633	67.336	-9.729	6.876	1.00	51.37
ATOM	4890	CD	GLU	633	66.490	-9.404	5.622	1.00	54.30
ATOM	4891	OE1	GLU	633	65.859	-8.327	5.523	1.00	55.85
ATOM	4892	OE2	GLU	633	66.460	-10.256	4.710	1.00	55.95
MOTA	4893	C	GLU	633	65.919	-9.592	9.677	1.00	42.72
MOTA	4894	0	GLU	633	65.360	-10.582	9.222	1.00	45.10
ATOM	4895	N	ASP	634	66.287	-9.494	10.949	1.00	42.83
MOTA	4897	CA	ASP	634	66.075	-10.585	11.884	1.00	43.03
ATOM	4898	CB	ASP	634	67.324	-10.809	12.743	1.00	49.02
ATOM	4899	CG	ASP	634	68.539	-11.240	11.916	1.00	55.95
ATOM	4900	OD1	ASP	634	68.462	-12.292	11.237	1.00	59.10
ATOM	4901	OD2	ASP	634	69.568	-10.525	11.943	1.00	59.41
MOTA	4902	С	ASP	634	64.848	-10.340	12.751	1.00	41.75
MOTA	4903	0	ASP	634	64.737	-10.873	13.847	1.00	42.79
ATOM	4904	N	ASN	635	63.937	-9.508	12.257	1.00	42.51
ATOM	4906	CA	ASN	635	62.686	-9.186	12.939	1.00	42.53
ATOM	4907	CB	ASN	635	61.768	-10.417	12.992	1.00	45.07
MOTA	4908	CG	ASN	635	61.483	-10.985	11.624	1.00	46.54
ATOM	4909	OD1	ASN	635	60.868	-10.336	10.786	1.00	49.77
MOTA	4910	ND2	ASN	635	61.949	-12.192	11.383	1.00	49.29
MOTA	4913	С	ASN	635	62.801	-8.577	14.331	1.00	40.51
ATOM	4914	0	ASN	635	61.939	-8.800	15.187	1.00	41.80
ATOM	4915	N	VAL	636	63.844	-7.795	14.561	1.00	37.98
ATOM	4917	CA	VAL	636	64.016	-7.164	15.856	1.00	33.92
ATOM	4918	CB	VAL	636	65.517	-7.005	16.195	1.00	32.21
ATOM	4919	CG1	VAL	636	65.697	-6.284	17.530	1.00	31.40
MOTA	4920	CG2	VAL	636	66.169	-8.367	16.242	1.00	30.93
MOTA	4921	С	VAL	636	63.349	-5.797	15.811	1.00	31.85
MOTA	4922	0	VAL	636	63.531	-5.061	14.849	1.00	33.47
MOTA	4923	N	MET	637	62.525	-5.492	16.807	1.00	31.69
ATOM	4925	CA	MET	637	61.860	-4.194	16.879	1.00	31.44
MOTA	4926	CB	MET	637	60.642	-4.241	17.820	1.00	34.97
MOTA	4927	CG	MET	637	59.559	-5.264	17.455	1.00	36.80
ATOM	4928	SD	MET	637	58.860	-5.048	15.803	1.00	35.45
ATOM	4929	CE	MET	637	59.030	-6.709	15.116	1.00	32.12
ATOM	4930	C	MET	637	62.874	-3.209	17.454	1.00	31.86
MOTA	4931	0	MET	637	63.512	-3.496	18.479	1.00	29.47
MOTA	4932	N	LYS	638	62.985	-2.041	16.820	1.00	30.87
MOTA	4934	CA	LYS	638	63.915	-0.994	17.244	1.00	29.66
ATOM	4935	CB	LYS	638	65.161	-0.983	16.349	1.00	27.51
MOTA	4936	CG	LYS	638	66.171	-2.059	16.691	1.00	27.29
ATOM	4937	CD	LYS	638	67.370	-1.984	15.781	1.00	28.55
ATOM	4938	CE	LYS	638	68.409	-3.029	16.150	1.00	24.75
MOTA	4939	NZ	LYS	638	68.964	-2.785	17.498	1.00	25.59
ATOM	4943	C	LYS	638	63.283	0.383	17.215	1.00	27.72
ATOM	4944	0	LYS	638	62.918	0.869	16.146	1.00	27.66
ATOM	4945	N	ILE	639	63.163	1.004	18.387	1.00	26.21
MOTA	4947	CA	ILE	639	62.597	2.343	18.501	1.00	26.27
MOTA	4948	CB	ILE	639	62.580	2.862	19.965	1.00	26.52
MOTA	4949	CG2	ILE	639	61.896	4.206	20.017	1.00	21.50
ATOM	4950	CG1	ILE	639	61.918	1.854	20.926	1.00	25.70
MOTA	4951	CD1	ILE	639	60.496	1.494	20.599	1.00	25.62

	ATOM	4952	С	TT 75									
	ATOM	4953	0	ILE	639	63.	505	3	.288	17			
	ATOM	4954	N	ILE	639		730		.281		.718	1.00	29.56
	ATOM	4956		ALA	640	62.	897	4	.101		. 906	1.00	27.74
	ATOM	4957	CA	ALA	640	63.	620	5	.071		857	1.00	
	ATOM	4958	CB	ALA	640	63.			.796		042	1.00	28.79
	ATOM	4959	C	ALA	640	63.	164				563	1.00	26.74
		4960	0	ALA	640	62.0	087		487	16.	385	1.00	28.91
		4962	N ~-	ASP	641	64.0			683		956	1.00	28.67
			CA	ASP	641	63.7			464	16.		1.00	28.25
		4963	CB	ASP	641	62.5			876	16.		1.00	30.80
		4964	CG	ASP	641	62.8	60		319	15.	128	1.00	33.44
	ma	4965	OD1		641	64.0	03		393	13.9	948	1.00	38.01
	ma		OD2		641	62.0	02		001	13.5	74	1.00	42.43
	ma		C		641	63.5	06		847	13.1	60	1.00	42.41
			0		541	63.0	0.1	9.3	311	17.7		1.00	41.74
			N	D	542	62.84	# /	10.3	809	18.0	_	1.00	29.07
			CA 1		42	64.13	88	8.6	04	18.6		1.00	28.42
		972 (	-		42	64.03	6	8.9	14	20.0		1.00	29.69
	COM 4	973 (			42	64.34	7	7.6	56	20.8	~ ~		29.62
		974 c			42 42	65.70	2	7.0		20.60		1.00	27.18
					42	66.84	8	7.5	59 2	21.23		1.00	23.96
		76 C			42	65.82	8	5. <b>9</b> ′	74 1	19.74			23.66
AT		77 C			42 42	68.090	0	6.99		0.98			24.08
AT		78 C	_	HE 64		67.069	9	5.40		9.50			23.02
AT		79 C				68.200		5.90		0.12	_		23.20
ATO		80 O				64.948		0.07		0.50			21.68
ATO			GI			64.755	. 1	0.66		1.57		.00	32.99
ATC						65.940	1	0.39		9.67			32.10
ATO			GL			66.869	1	1.46		0.003	-		4.66
ATO	M 498		GL			66.639	1:	2.75				.00 3	5.29
ATO	M 498		LE	·		67.464		3.666		9.250 9.333			9.13
ATO						65.520	12	2.850		.532			9.83
ATO	M 498		LE	<del>-</del> .		65.202	14	.043		745			2.26
ATO	499					63.935	13	.843		. /45		00 4	5.25
ATOM	1 499		LE			63.911	12	.839		.911	1.		1.59
ATOM						62.653	13	.068		.763	1.		3.00
ATOM	499					65.119		.016		.940	1.0	00 42	.61
ATOM		_	LEU			65.037		.298		.889	1.(	00 45	.65
ATOM		_	LEU		•	64.391	15	. 281		578	1.0	00 49	. 59
ATOM			ALA		6	55.585	16	401		623	1.0	0 51	. 90
ATOM	4998		ALA	645		5.495		677		080	1.0	0 52	- 08
ATOM	4999		ALA	645	6	6.414		699		777	1.0	0 54	. 71
MOTA	5000	0	ALA	645	6	4.053	18	184		124	1.0		. 38
MOTA	5001		ALA	645	6	3.534	18	582	18.		1.0	0 55.	44
ATOM	5003	N	ASP	652	5	2.389	21.	J02 E43	19.		1.0	0 56.	69
ATOM	5004	CA	ASP	652	5	1.207	21.	243	14.		1.00	73.	
ATOM	5005	CB	ASP	652	5:	1.601	21.	745	13.9		1.00	73.	
ATOM	5005	CG	ASP	652	50	0.398	21.9	775	12.4		1.00		
ATOM		OD1	ASP	652	49	3.354	22.2	74T	11.5		1.00	72.	
ATOM	5007	OD2	ASP	652	50	.497	22.7	/15	12.0	65	1.00		
ATOM	5008	C	ASP	652	50	.321	21.9	756	10.3	57	1.00		
ATOM	5009	0	ASP	652	50	.568	20.5	14	14.0	42	1.00		
ATOM	5010	N	TYR	653		.272	19.4	95	13.3	94	1.00	75.9	
ATOM	5012	CA	TYR	653			20.6		14.8		1.00	75.5	
TOM	5013	CB	TYR	653	40 17	.348	19.5		15.06	54	1.00		
CCCD/=-					4/	. 274	19.9		16.08		1.00	75.6 76.8	
SSSD/55	145. v01											, 0 . 8	J



1 00 1	79.55
47 771 19.995 17.313	80.89
ATOM 5014 CG 118 563 46.983 20.567 18.516 1.00	83.02
ATOM 5015 CD1 118 47.438 20.648 19.830	80.87
ATOM 5016 CE1 118 653 49.032 19.503 17.874 100	81.70
ATOM 5017 CD2 11R 05 49 496 19.578 19.183 1.00	83.09
ATOM 5018 CE2 TYR 633 48 698 20.152 20.160 1.00	83.73
ATOM 5019 CZ TYR 653	75.03
ATOM 5020 OH TYR 653 47.685 19.038 13.787 1.00	
ATOM 5022 C TYR 653 17.897 13.711 1.00	75.97
TOM 5023 O TYR 653 19 885 12.767 1.00	73.85
ATOM 5024 N TYR 654 47.038 19.538 11.507 1.00	73.32
TYR 654 47.03 20 750 10.972 1.00	71.97
TYR 654 46.27 21 276 11.954 1.00	70.94
ATTOM 5028 CG TYR 654 45.250 21.801 13.185 1.00	71.41
The second secon	73.60
TYR 654 44.733 11.600 1.00	71.81
TVR 654 43.899 22.10 1.00	74.81
ATOM 5032 TVR 654 42.956 21.042 13.832 3.00	74.84
ATOM 302 TVR 654 43.380 22.132 14.769 1.00	76.60
ATOM 5055 CH TVR 654 42.457 22.572 20.446 1.00	73.82
ATOM 3034 0 TVR 654 47.975 18.30 2.29 1.00	74.25
ATOM 3037 0 TVR 654 47.545 18.671 10.784 1.00	74.04
ATOM 5037 1 LVS 655 49.249 18.500 2 927 1.00	75.41
ATOM 3030 CD 1.VS 655 50.195 18.230 16.4 1.00	78.45
ATOM 5045 GP LVS 655 51.626 18.000 2.151 1.00	83.01
ATOM 3041 70 1VS 655 52.647 18.198 2 527 1 00	
ATOM 5042 CG 125 655 54.062 18.589 9.537 1.00	
ATOM 5043 CD 222 CEE 55.076 17.813 8.703	
ATOM 5044 CE 113 56.489 18.133 9.074	
ATOM 5045 NZ 222 CSE 50.075 16.736 9.832	
ATOM 5049 C 55 50.245 16.092 10.872	
ATOM 5050 U BIS 656 49.750 16.173 8.872 1.00	_
ATOM 5051 N 110 656 49.597 14.730 8.533 1.00	
ATOM 5053 CA 110 656 48.723 14.406 7.323 1.00	
ATOM 5054 CB 113 656 47.266 14.753 7.519 1.00	
ATOM 5055 CG BIS 656 46.489 14.535 6.239 1.00	
ATOM 5056 CD LYS 656 45 001 14.655 6.483 1.00	
ATOM 5057 CE LYS 636 14.637 5.204 1.0	and the second s
ATOM 5058 NZ LYS 636 50 839 14.016 8.414 1.0	_
ATOM 5062 C LYS 636 51 804 14.578 7.897 1.0	-
ATOM 5063 O LYS 656 49 137 9.764 5.736 1.0	
ATOM 5064 N GLY 660 48 106 10.781 5.848 1.0	
ATOM 5066 CA GLY 660 47 407 10.761 7.192 1.0	_
ATOM 5067 C GLY 860 16 289 11.263 7.328 1.0	
ATOM 5068 O GLY 660 10.163 8.183 1.0	
ATOM 5069 N ARG 661 40 10.083 9.527 1.0	
ATOM 5071 CA ARG 661 1 9 799 10.229 1.1	00 51.79
ATOM 5072 CB ARG 661 47.542 7.523 9.450 1.	00 50.59
ATOM 5073 CG ARG 661 47.883 6 323 10.367 1.	00 53.68
ATOM 5074 CD ARG 661 47.822 5.044 9.665 1.	00 52.66
NTOM 5075 NE ARG 661 47.714 3.863 10.236 1.	00 51.73
27 ARG 661 47.920 11 518 1.	00 50.23
A10M 307 ARG 661 48.264 3.794 1	00 52.58
A10M 30 ARG 661 47.800 2.731	.00 44.80
A10M 3001 C ARG 661 47.915 11.23	.00 43.61
A10M 300 APG 661 48.865 11.998	
ATOM 5085 O ARG 001	

							Т.	82					
	ATOM	5086	N	LEU	663								
	ATOM	5088	CA	LEU	662		221	11	.528	11	.453		
	ATOM	5089	CB		662	47.	518		.654			1.00	40.74
	ATOM	5090	CG	LEU	662	46.	234		.415		.333	1.00	37.88
	ATOM	5091		LEU	662	45.	515	14	.074		671	1.00	36.19
	ATOM	5092	CD1		662	44.(		3.4	.074		499	1.00	35.32
	ATOM		CD2	LEU	662	46.2	777		.278		831	1.00	31.05
		5093	C		662	40.2	C 2		.383	11.	156	1.00	
	7 m	5094	0		662	48.1	.62		170		622	1.00	34.37
		5095	N		663	47.5	29	11.	479	14.			35.34
7	MOTA	5096	CD			49.4	41	12.	518	13.		1.00	33.06
7	MOTA	5097	CA	`	63	50.3		13.	113			1.00	36.39
A		5098			63	50.1	58	12.	107	12.		1.00	37.57
		5099	CB		63	51.5	16	12.	707	15.0		1.00	36.39
			CG	PRO 6	63	51.7	20	12.	787	14.8	85	1.00	36.98
			C	PRO 6	63	49.47	. 0	12.6		13.4	01	1.00	20.30
			0		63	49.4	, ,	12.4	191	16.3		1.00	38.48
	TOM 5	102		_	54	49.69		11.8		17.3			35.47
	rom 5	104 (		-	54	48.64	6	13.5		16.3		1.00	35.08
	rom 5					47.95	1	13.9				1.00	34.28
A			<b>.</b>			47.03	8	15.1		17.5		1.00	34.43
ΑT			·	AL 66	4	47.88		16.4		17.3°		1.00	36.92
				'AL 66	4	46.09				17.16			37.55
			•	'AL 66	4	47.13		14.9		16.18			38.28
AT		109 0	v	AL 66	4	46.908		12.74	19 1	8.12			33.03
		.10 N	L	YS 66		40.908		12.64	1 1	9.31			
AT	• • •	.12 C	A L	YS 66		46.803		.1.80	9 1	7.23			34.62
AT		13 C	_	YS 66		46.040	) 1	0.63		7.61			2.47
AT(		14 C	_			45.456		9.95		6.37	_		0.71
ATO	DM 51					44.324	1	0.77					9.59
ATO	DM 51:					43.927		0.33		5.76		00 2	9.64
ATC	M 51					42.664		1.05		1.36°			1.86
ATO						42.296	1/	0.72		8.899			0.42
ATO			LY	S 665		46.801				.486			5.50
ATO		_	LY	S 665		46.230		9.644		.498		00 32	2.23
ATO			TR	P 666		49 000		3.659		. 955	1.	_	0.04
			TR			48.080		.915	18	.748			7.04
ATO		6 CB	TRI			48.886		.068	19	.619			38
ATON		7 CG	TRI			50.204	8	.682		. 945			.32
ATON		B CD2				50.078		.530		.006	1.0		.07
ATOM	1 5129	9 CE2				49.531		. 559		684	1.0		.26
ATOM						49.630		.257			1.0	<b>-</b> .	.07
ATOM	513]					48.982		569		163	1.0		. 71
ATOM						50.473				882	1.0	0 26	
ATOM			TRP	666		0.206	٥.	238		234	1.0	0 24.	
ATOM	1		TRP	666		9.190	5.	469	17.	132	1.0		
	5135		TRP	666	7	9.540	5.	929	14.	874	1.0		
ATOM	5136	CH2	TRP	666	7	8.548	8.	248	14.	599	1.0		22
ATOM	5137	С	TRP			8.658	6.	934	14.			- •	14
ATOM	5138	0	TRP	666		9.203		802	20.9		1.00		
ATOM	5139	N		666	4	9.688		202			1.00		84
ATOM	5141		MET	667		8.905			21.8		1.00	32.	82
ATOM		CA	MET	667	4	9.180	11.0	777	20.9		1.00	35.	
	5142	CB	MET	667	4	9.150	11.9	160	22.0		1.00	•	
ATOM	5143	CG	MET	667	Z.		13.4	123	21.6		1.00		
ATOM	5144	SD	MET	667	٦ ( - م	.487	13.9		21.2	26	1.00		
ATOM	5145	CE	MET		50	384	15.7		20.9				
ATOM	5146	C	MET	667		711	15.7	45	19.1		1.00	-	
ATOM	5147	ō		667	48	.294	11.8	02			1.00	49.2	
ATOM	5148		MET	667		.066	11.6		23.28		1.00	38.9	8
-		N	ALA	668	48	. 933	11 0		23.18	33	1.00	39.1	8
SSSD/55	145				-		11.8	44	24.45	56	1.00	38.7	2
222D/35	145. V01											/ .	-





MOTA 5150 CA ALA 668 48.231 11.728 25.727 1.00 37.82 MOTA 5151 CB ALA 668 49.224 11.527 26.857 1.00 38.49 MOTA 5152 C ALA 668 47.497 13.051 25.891 1.00 38.16 **ATOM** 5153 0 ALA 668 47.937 14.072 25.363 1.00 37.21 **ATOM** 5154 N PRO 669 46.383 13.062 26.644 1.00 39.78 **ATOM** 5155 CD PRO 669 45.785 11.931 27.367 1.00 40.08 MOTA 5156 CA **PRO** 669 45.598 14.281 26.858 1.00 40.68 MOTA 5157 CB PRO 669 44.474 13.806 27.782 1.00 42.15 MOTA 5158 CG PRO 669 44.346 12.352 27.446 1.00 42.56 ATOM 5159 С PRO 669 46.398 15.432 27.484 1.00 42.69 **ATOM** 5160 0 PRO 669 46.320 16.566 27.019 1.00 42.14 **ATOM** 5161 N GLU 670 47.168 15.153 28.532 1.00 43.21 MOTA 5163 CA GLU 670 47.956 16.211 29.160 1.00 44.62 MOTA 5164 CB GLU 670 48.651 15.719 30.429 1.00 44.95 MOTA 5165 CG GLU 670 49.824 14.782 30.197 1.00 45.54 ATOM 5166 CD GLU 670 49.422 13.332 30.079 1.00 42.72 ATOM 5167 OE1 GLU 670 50.332 12.481 30.066 1.00 41.43 ATOM 5168 OE<sub>2</sub> GLU 670 13.036 48.212 30.015 1.00 44.44 **ATOM** 5169 С GLU 670 48.993 16.772 28.195 1.00 44.88 ATOM 5170 0 GLU 670 49.248 17.968 28.194 1.00 45.08 **ATOM** 5171 N ALA 671 49.565 15.908 27.358 1.00 44.75 ATOM 5173 CA ALA 671 50.573 16.323 26.392 1.00 45.92 ATOM 5174 CB ALA 671 51.256 15.095 25.766 1.00 44.10 ATOM 5175 C ALA 671 49.944 17.193 25.314 1.00 47.96 ATOM 5176 0 ALA 671 50.526 18.192 24.894 1.00 49.16 MOTA 5177 N LEU 672 48.729 16.836 24.917 1.00 49.84 **ATOM** 5179 CA LEU 672 47.989 17.554 23.881 1.00 50.74 ATOM 5180 CB LEU 672 46.926 16.619 23.289 1.00 53,20 **ATOM** 5181 CG LEU 672 46.184 16.989 22.004 1.00 55.26 **ATOM** 5182 CD1 LEU 672 47.153 17.155 20.856 1.00 57.12 ATOM 5183 CD2 LEU 672 45.203 15.895 21.680 1.00 52.86 **ATOM** 5184 C LEU 672 47.327 18.826 24.408 1.00 50.79 MOTA 5185 0 LEU 672 47.302 19.855 23.736 1.00 50.95 ATOM 5186 PHE N 673 46.792 18.751 25.618 1.00 52.07 MOTA 5188 PHE CA 673 46.111 19.884 26.226 1.00 54.39 MOTA 5189 CB PHE 673 44.892 19.396 27.019 1.00 51.21 ATOM 5190 CG PHE 673 43.871 18.656 26.186 1.00 48.49 **ATOM** 5191 CD1 PHE 673 43.304 17.473 26.646 1.00 47.79 ATOM 5192 CD2 PHE 673 43.470 19.149 24.949 1.00 49.04 MOTA 5193 CE1 PHE 673 42.349 16.789 25.888 1.00 47.90 MOTA 5194 CE2 PHE 673 42.511 18.473 24.182 1.00 49.71 ATOM 5195 PHE CZ673 41.952 17.288 24.655 1.00 46.86 ATOM 5196 PHE С 673 47.007 20.741 27.123 1.00 58.25 **ATOM** 5197 PHE 673 0 47.000 21.971 27.034 1.00 60.52 ATOM 5198 N ASP 674 47.784 20.094 27.983 1.00 59.63 **ATOM** 5200 **ASP** CA 674 48.652 20.815 28.905 1.00 62.11 MOTA 5201 CB ASP 674 48.568 30.307 20.196 1.00 63.81 **ATOM** 5202 ASP CG 674 47.143 20.015 30.791 1.00 66.46 MOTA 5203 OD1 ASP 674 46.815 18.901 31.247 1.00 66.70 MOTA 5204 OD2 ASP 674 46.354 20.981 30.722 1.00 68.77 ATOM 5205 C ASP 674 50.119 20.852 28.482 1.00 63.36 ATOM 5206 0 ASP 674 50.979 21.175 29.310 1.00 64.11 **ATOM** 5207 N ARG 675 50.410 20.486 27.228 1.00 62.94

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5209

CA

ARG

675

51.789

20.456

26.706

1.00

60.75

**ATOM** 

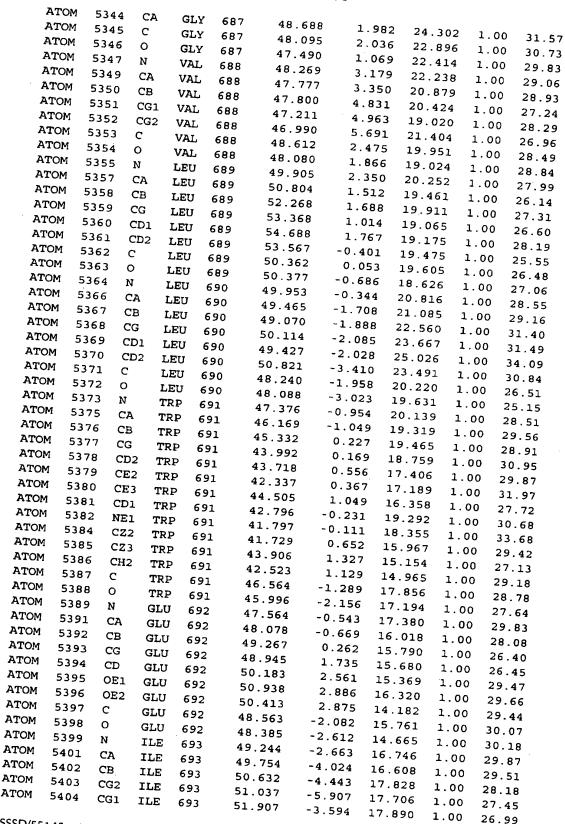




_					104		
ATO		CB	ARG 67	5 50 05			
ATO			ARG 67	~2.2,			1.00 60.56
ATO			ARG 67	/			1.00 63.67
ATON			ARG 67				1.00 66.99
ATOM	5215		ARG 679	23.30		24.337	
ATOM	5216			34.00		24.173	
ATOM			_	22.03	7 26.254	24.590	
ATOM		_	RG 675	25	24.965	23.593	1.00 65.81
ATOM	F005		RG 675		19.793	27.700	1.00 68.76
ATOM			RG 675	53.933	20.130	27.766	1.00 58.06
ATOM			LE 676		18.859		1.00 59.30
ATOM			LE 676	52.992	18.141	28.483	1.00 55.62
ATOM			LE 676	52.154		29.489	1.00 54.09
ATOM	~ ~		E 676	52.749		30.765	1.00 52.69
		CG1 II		52.049		31.629	1.00 49.38
ATOM		D1 II		51.306		31.540	1.00 53.15
ATOM	5231 C	: II			19.103	32.845	1.00 57.79
MOTA	5232 C			53.468	16.796	28.953	
ATOM	5233 N			52.668	15.891	28.730	• • •
ATOM	5235 C			54.773	16.671	28.745	
ATOM	5236 C			55.343	15.436		1.00 51.76
ATOM	5237 C			56.232	15.722		1.00 49.42
ATOM	E000			55.466		0 =	1.00 51.33
ATOM				55.158			1.00 56.22
ATOM	~	- <b></b>		54.491		<b>.</b>	1.00 56.12
ATOM				55.078		24.479	1.00 56.18
ATOM			677	54.411			1.00 58.13
ATOM	5242 CZ			54.125			L.00 57.65
ATOM	5243 OH	TYR	677	53.504		23.512	00 58.23
_	5245 C	TYR	677	56.136		22.360 1	00 61.71
	5246 O	TYR	677	56.983		29.316 1	.00 46.46
	5247 N	THR		55.818		29.970 1	.00 48.65
	5249 CA	THR	678		13.464 2	9.537 1	.00 41.73
	5250 CB	THR	678	56.498	12.664 3		.00 39.83
	5251 OG:	THR	678	55.680	12.593 3		.00 41.78
	5253 CG2		678	54.462	11.867 3		.00 45.77
ATOM 9	254 C	THR		55.342		_	
3	255 o	THR	678	56.661		0 0	
ATOM 5	256 N	HIS	678	56.258		_	10
	258 CA		679	57.264		_	· <del></del>
3	259 CB	HIS	679	57.423			00 36.36
30000		HIS	679	58.348	_		00 35.91
		HIS	679	59.761	0		00 35.05
		HIS	679	60.453		404 1.	400
		HIS	679	60.632	A ===	2.278 1.	
	264 CE1	HIS	679	61.803	_	.380 1.	00 37.49
3.	265 NE2	HIS	679	61.721		.621 1.	00 39.58
	267 C	HIS	679	56.032		.766 1.0	
3	268 O	HIS	679	55.771		.441 1.0	
	69 N	GLN	680		7.458 29	.660 1.0	00 37.16
ATOM 52	71 CA	GLN	680	55.126	8.908 31	.264 1.0	_
	72 CB	GLN		53.754		.332 1.0	2,
ATOM 52			680	53.069		640 1.0	_ ~
ATOM 52			680	53.645		884 1.0	
ATOM 52			680	53.676			
ATOM 52			680	52.669	_	-	
3.000	<b></b>		680	54.846			
ATOM 52	79 C	GLN (			0 0	464 1.0	
SSSD/EE14-	0.4				044 30.	121 1.0	0 37.54
SSSD/55145.	VU1						



MOTA	5280	0	GLN	680	51.950	8.185	29.765	1.00	37.93
ATOM	5281	N	SER	681	53.282	9.961	29.504	1.00	36.38
ATOM	5283	CA	SER	681	52.563	10.367	28.306	1.00	38.05
ATOM	5284	CB	SER	681	52.857	11.819	27.940	1.00	41.41
ATOM	5285	OG	SER	681	54.239	12.069	27.938	1.00	42.92
ATOM	5287	C	SER	681	52.991	9.421	27.178	1.00	37.92
ATOM	5288	0	SER	681	52.205	9.148	26.263	1.00	37.21
ATOM	5289	И	ASP	682	54.237	8.932	27.248	1.00	34.77
ATOM	5291	CA	ASP	682	54.750	7.972	26.267	1.00	31.99
MOTA	5292	CB	ASP	682	56.243	7.683	26.481	1.00	31.08
ATOM	5293	CG	ASP	682	57.165	8.638	25.721	1,00	33.63
MOTA	5294	OD1	ASP	682	58.386	8.503	25.920	1.00	32.35
ATOM	5295	OD2	ASP	682	56.707	9.500	24.930	1.00	29.46
MOTA	5296	C	ASP	682	53.969	6.672	26.457	1.00	31.54
ATOM	5297	0	ASP	682	53.675	5.971	25.493	1.00	29.94
ATOM	5298	N	VAL	683	53.677	6.334	27.712	1.00	30.48
ATOM	5300	CA	VAL	683	52.913	5.126	28.023	1.00	32.94
ATOM	5301	CB	VAL	683	52.731	4.939	29.572	1.00	33.94
ATOM	5302	CG1	VAL	683	51.635	3.905	29.872	1.00	32.71
ATOM	5303	CG2	VAL	683	54.042	4.474	30.209	1.00	27.41
ATOM	5304	C	VAL	683	51.545	5.164	27.299	1.00	32.27
ATOM	5305	0	VAL	683	51.106	4.158	26.733	1.00	30.54
ATOM ATOM	5306	N	TRP	684	50.902	6.332	27.282	1.00	32.57
ATOM	5308	CA	TRP	684	49.616	6.477	26.600	1.00	32.76
MOTA	5309 5310	CB CG	TRP	684 684	49.060	7.895	26.765	1.00	33.67
ATOM	5310	CD2	TRP TRP	684	47.855	8.210	25.891	1.00	38.22
ATOM	5311	CE2	TRP	684	46.503	8.435	26.328	1.00	39.96
ATOM	5312	CE3	TRP	684	45.734	8.735	25.177	1.00	39.59
ATOM	5313	CD1	TRP	684	45.869	8.416.		1.00	39.26
ATOM	5315	NE1	TRP	684	47.842 46.576	8.373 8.687	24.528 24.096	1.00 1.00	39.02
ATOM	5317	CZ2	TRP	684	44.362	9.011	25.240	1.00	38.42 36.62
ATOM	5318	CZ3	TRP	684	44.502	8.691	27.641	1.00	40.70
ATOM	5319	CH2	TRP	684	43.766	8.982	26.475	1.00	40.57
ATOM	5320	C	TRP	684	49.819	6.158	25.125	1.00	31.98
ATOM	5321	0	TRP	684	49.066	5.367	24.557	1.00	32.43
ATOM	5322	N	SER	685	50.859	6.748	24.529	1.00	29.63
ATOM	5324	CA	SER	685	51.195	6.531	23.119	1.00	28.62
ATOM	5325	CB	SER	685	52.457	7.296	22.751	1.00	24.72
ATOM	5326	OG	SER	685	52.323	8.664	23.072	1.00	30.04
MOTA	5328	С	SER	685	51.414	5.055	22.825	1.00	27.91
ATOM	5329	0	SER	685	51.022	4.555	21.767	1.00	28.60
ATOM	5330	N	PHE	686	52.063	4.372	23.763	1.00	27.96
ATOM	5332	CA	PHE	686	52.333	2.947	23.662	1.00	27.03
MOTA	5333	CB	PHE	686	53.163	2.499	24.868	1.00	25.79
ATOM	5334	CG	PHE	686	53.440	1.029	24.890	1.00	26.25
ATOM	5335	CD1	PHE	686	54.252	0.451	23.923	1.00	27.32
MOTA	5336	CD2	PHE	686	52.839	0.208	25.841	1.00	26.22
ATOM	5337	CE1	PHE	686	54.464	-0.930	23.900	1.00	25.87
ATOM	5338	CE2	PHE	686	53.046	-1.170	25.828	1.00	24.37
MOTA	5339	CZ	PHE	686	53.856	-1.740	24.854	1.00	26.42
MOTA	5340	С	PHE	686	51.003	2.160	23.596	1.00	28.82
ATOM	5341	0	PHE	686	50.912	1.129	22.914	1.00	26.74
MOTA	5342	N	GLY	687	49.991	2.636	24.324	1.00	29.52



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MOTA	5405	CD1	ILE	693	52.663	-3.747	19.194	1.00	25.37
MOTA	5406	С	ILE	693	48.603	-5.023	16.452	1.00	29.21
ATOM	5407	0	ILE	693	48.568	-5.807	15.512	1.00	27.89
MOTA	5408	N	PHE	694	47.623	-4.942	17.336	1.00	31.33
ATOM	5410	CA	PHE	694	46.523	-5.888	17.279	1.00	34.41
ATOM	5411	CB	PHE	694	45.958	-6.114	18.687	1.00	35.37
MOTA	5412	CG	PHE	694	46.978	-6.717	19.621	1.00	35.60
MOTA	5413	CD1	PHE	694	47.606	-5.942	20.586	1.00	37.23
MOTA	5414	CD2	PHE	694	47.424	-8.024	19.426	1.00	35.59
ATOM	5415	CE1	PHE	694	48.669	-6.460	21.333	1.00	36.39
MOTA	5416	CE2	PHE	694	48.484	-8.546	20.170	1.00	35.34
ATOM	5417	CZ	PHE	694	49.110	-7.762	21.118	1.00	35.71
ATOM	5418	C	PHE	694	45.481	-5.715	16.176	1.00	34.41
MOTA	5419	0	PHE	694	44.623	-6.579	15.982	1.00	34.48
ATOM	5420	N	THR	695	45.617	-4.637	15.404	1.00	33.03
MOTA	5422	CA	THR	695	44.742	-4.379	14.263	1.00	31.81
MOTA	5423	CB	THR	695	44.113	-2.957	14.278	1.00	29.75
MOTA	5424	OG1	THR	695	45.142	-1.961	14.218	1.00	30.72
MOTA	5426	CG2	THR	695	43.254	-2.759	15.524	1.00	29.40
MOTA	5427	С	THR	695	45.596	-4.533	13.011	1.00	31.44
MOTA	5428	0	THR	695	45.153	-4.241	11.906	1.00	33.00
MOTA	5429	N	LEU	696	46.832	-4.987	13.209	1.00	31.24
ATOM	5431	CA	LEU	696	47.799	-5.199	12.134	1.00	31.36
MOTA	5432	CB	LEU	696	47.421	-6.418	11.291	1.00	33.53
MOTA	5433	CG	LEU	696	47.270	-7.741	12.042	1.00	33.00
MOTA	5434	CD1	LEU	696	47.010	~8.838	11.052	1.00	35.50
MOTA	5435	CD2	LEU	696	48.515	-8.061	12.830	1.00	36.09
ATOM	5436	C	LEU	696	48.066	-3.976	11.249	1.00	30.84
MOTA	5437	0	LEU	696	48.135	-4.067	10.024	1.00	28.23
ATOM	5438	N	GLY	697	48.302	-2.839	11.890	1.00	31.54
ATOM	5440	CA	GLY	697	48.591	-1.632	11.141	1.00	33.87
ATOM	5441	С	GLY	697	47.375	-0.765	10.924	1.00	32.77
MOTA	5442	0	GLY	697	47.322	0.042	9.994	1.00	33.90
ATOM	5443	N	GLY	698	46.392	-0.921	11.797	1.00	33.29
ATOM	5445	CA	GLY	698	45.187	-0.122	11.681	1.00	32.66
ATOM	5446	C	GLY	698	45.408	1.368	11.877	1.00	30.57
ATOM	5447	0	GLY	698	46.336	1.803	12.553	1.00	27.36
ATOM	5448	N	SER	699	44.517	2.148	11.285	1.00	30.92
ATOM	5450	CA	SER	699	44.552	3.595	11.376	1.00	32.19
MOTA	5451	CB	SER	699	44.062	4.202	10.058	1.00	34.24
ATOM	5452	og	SER	699	44.019	5.616	10.123	1.00	38.67
ATOM	5454	C	SER	699	43.644	4.014	12.538	1.00	31.81
MOTA	5455	0	SER	699	42.431	3.759	12.525	1.00	31.39
ATOM	5456	N	PRO	700	44.228	4.597	13.594	1.00	31.82
ATOM	5457	CD	PRO	700	45.645	4.842	13.919	1.00	28.82
ATOM	5458	CA	PRO	700	43.353	4.992	14.697	1.00	31.31
ATOM	5459	CB	PRO	700	44.345	5.341	15.809	1.00	31.31
ATOM	5460	CG	PRO	700	45.552	5.800	15.061	1.00	30.41
ATOM	5461	C	PRO	700	42.484	6.170	14.295	1.00	31.19
ATOM	5462	0	PRO	700	42.899	7.021	13.510	1.00	29.93
ATOM	5463	N	TYR	701	41.235	6.144	14.736	1.00	32.69
ATOM	5465	CA	TYR	701	40.291	7.223	14.445	1.00	32.54
ATOM	5466	CB	TYR	701	40.650	8.416	15.323	1.00	34.47
MOTA	5467	CG	TYR	701	40.512	8.141	16.794	1.00	39.16

70.											
		5468	CD1	TYR	701	41.5	42 0	425			
		5469	CE1	TYR	701				7.683	1.00	44.31
		470	CD2	TYR	701		_		9.060	1.00	46.65
		471.	CE2	TYR	701	٠,٠,٠			1.307	1.00	41.21
		472	CZ	TYR	701	93.19		447 18	.657	1.00	45.05
	TOM 5	473	OH	TYR	701	-0.40	•	750 19	. 535	1.00	47.24
A7	rom 5		_	TYR		39.94			. 886	1.00	
A		4	_	TYR	701	40.21			. 972	1.00	52.18
AT					701	40.37			.647	1.00	30.56
				PRO	702	39.92	8 6.		.058		29.73
		`		PRO	702	39.65	9 5.2		. 261	1.00	30.38
		`		PRO	702	39.84	7 7.0		642	1.00	30.22
AT				PRO	702	39.69				1.00	28.87
AT				PRO	702	39.00		-	948	1.00	29.63
		82 C	_	PRO	702	38.722			959	1.00	30.99
ATO	-··	83 C	) F	PRO	702	37.557			283	1.00	30.88
AT(		84 N	G	LY	703	39.100			636	1.00	33.98
ATO		86 C	A G	LY	703	38.154	. —	16 9.	584	1.00	29.03
ATC		87 C		LY	703			34 9.	169	1.00	28.98
ATC	DM . 54	88 O		LY	703	37.893		59 10.:		1.00	29.69
ATC		89 N			704	37.074		58 10.6	_	1.00	31.71
ATO		91 C			704	38.579		10 11.3		1.00	
ATO	M 549					38.416	11.95	12.5			30.74
ATO	M 549		• •		704	38.582	11.20	8 13.8			32.06
ATO					704	38.522	12.19	7 15.0			31.70
ATO!					704	37.506	10.14				30.29
ATO			VA		704	39.430	13.08				31.56
ATO		_	VA		704	40.634	12.86				33.72
ATON		_	PR		05	38.957	14.30			.00	35.31
ATOM					05	37.594	14.69	_			34.23
ATOM			PR		05	39.875	15.44			.00 3	33.20
ATOM			PR	0 7	05	39.053	16.49			.00 3	3.73
ATOM			PR	7	05	37.647	16.187				4.93
ATOM		. •	PRO	7	05	40.280	15.879			.00 3	6.93
			PRO	7	05	39.651			-	.00 з	3.25
ATOM			VAI	7	06	41.322	15.490				1.71
ATOM			VAI	. 70	06	41.852	16.697				4.46
ATOM	5507	CB	VAL		06	42.923	17.176				6.99
ATOM	5508	CG1	VAL			43.577	18.261	14.68			9.01
ATOM	5509	CG2					18.618	16.01			0.33
ATOM	5510	C	VAL			43.961	17.786	13.67			3.61
ATOM	5511	0	VAL			40.826	17.716	15.89	51.		5.65
ATOM	5512	N	GLU			40.823	17.319	17.06			3.55
ATOM	5514	CA	GLU	70		39.955	18.605	15.426	5 1.		.74
ATOM	5515	СВ	GLU			38.941	19.220	16.278	3 1.		
ATOM	5516	C		70		38.129	20.242	15.482			.20
ATOM	5517	ō	GLU	70		38.014	18.188	16.900			. 98
ATOM	5518	N	GLU	70		37.634	18.295	18.074			.46
ATOM	5520		GLU	708		37.681	17.170	16.115			.04
ATOM	5521	CA	GLU	708		36.802	16.105	16.571			.81
ATOM		CB	GLU	708	3	36.316	15.289				.70
ATOM	5522 5522	CG	GLU	708	1	35.459	16.091	15.378			
	5523	CD	GLU	708		34.235	16.677	14.413			. 44
ATOM	5524	OE1	GLU	708		33.629		15.084	1.0	0 51.	
ATOM	5525	OE2	GLU	708		33.882	16.007	15.961	1.0	0 50.	
ATOM	5526	C	GLU	708		37.506	17.824	14.732	1.0		
ATOM	5527	0	GLU	708			15.223	17.588	1.0		
					•	36.897	14.782	18.567	1.0		
SSSD/55	145 vn1									~ .	-0

WO 98/07835



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ATOM	5528	N	LEU	709	38.799	14.993	17.376	1.00	35.69
ATOM	5530	CA	LEU	709	39.584	14.179	18.301	1.00	35.48
MOTA	5531	CB	LEU	709	41.039	14.044	17.830	1.00	34.84
MOTA	5532	CG	LEU	709	41.921	13.250	18.802	1.00	32.41
ATOM	5533	CD1	LEU	709	41.608	11.787	18.674	1.00	30.10
MOTA	5534	CD2	LEU	709	43.378	13.514	18.560	1.00	29.93
MOTA	5535	C	LEU	709	39.568	14.842	19.673	1.00	35.58
MOTA	5536	0	LEU	709	39.377	14.177	20.694	1.00	35.43
ATOM	5537	N	PHE	710	39.792	16.150	19.686	1.00	36.79
ATOM	5539	CA	PHE	710	39.800	16.918	20.927	1.00	40.58
ATOM	5540	CB	PHE	710	39.944	18.413	20.637	1.00	42.55
MOTA	5541	CG	PHE	710	41.308	18.808	20.162	1.00	46.38
ATOM	5542	CD1	PHE	710	42.392	17.942	20.313	1.00	47.29
MOTA	5543	CD2	PHE	710	41.515	20.050	19.580	1.00	47.93
MOTA	5544	CEI	PHE	710	43.659	18.312	19.892	1.00	51.21
MOTA	5545	CE2	PHE	710	42.781	20.435	19.155	1.00	50.89
MOTA	5546	CZ	PHE	710	43.859	19.562	19.312	1.00	53.31
MOTA	5547	C	PHE	710	38.517	16.676	21.694	1.00	40.14
MOTA	5548	0	PHE	710	38.543	16.446	22.898	1.00	39.86
ATOM	5549	N Ca	LYS	711	37.399 36.101	16.705	20.977	1.00	41.02
MOTA	5551	CA	LYS	711	30.101	16.479	21.584	1.00	38.66
ATOM	5552	CB	LYS	711	34.985	16.803	20.580	1.00	40.75
ATOM	5553	CG	LYS	711	33.601	16.727	21.181	1.00	46.99
ATOM ATOM	5554 5555	CD CE	LYS	711	32.522	17.174	20.218	1.00	50.71
ATOM	5556	NZ	LYS LYS	711 711	31.163	16.733	20.739	1.00	52.53
ATOM	5560	C	LYS	711	30.041 35.990	17.194 15.046	19.884 22.120	1.00	57.76 38.06
ATOM	5561	0	LYS	711	35.535	14.831	23.250	1.00	
ATOM	5562	N	LEU	712	36.431	14.066	21.330	1.00	36.29 38.10
ATOM	5564	CA	LEU	712	36.392	12.662	21.764	1.00	38.69
ATOM	5565	CB	LEU	712	36.914	11.714	20.672	1.00	37.19
ATOM	5566	CG	LEU	712	36.070	11.436	19.424	1.00	34.73
ATOM	5567	CD1	LEU	712	36.814	10.453	18.524	1.00	35.54
ATOM	5568	CD2	LEU	712	34.709	10.872	19.818	1.00	30.90
ATOM	5569	С	LEU	712	37.230	12.472	23.021	1.00	39.62
ATOM	5570	0	LEU	712	36.843	11.745	23.940	1.00	39.44
ATOM	5571	N	LEU	713	38.398	13.101	23.044	1.00	40.10
MOTA	5573	CA	LEU	713	39.279	12.999	24.199	1.00	42.81
MOTA	5574	CB	LEU	713	40.606	13.716	23.924	1.00	41.70
ATOM	5575	CG	LEU	713	41.495	13.040	22.868	1.00	41.86
ATOM	5576	CD1	LEU	713	42.742	13.862	22.607	1.00	37.19
ATOM	5577	CD2	LEU	713	41.873	11.647	23.340	1.00	41.17
MOTA	5578	С	LEU	713	38.577	13.566	25.437	1.00	43.18
MOTA	5579	0	LEU	713	38.479	12.889	26.457	1.00	44.79
MOTA	5580	N	LYS	714	38.004	14.760	25.312	1.00	42.75
MOTA	5582	CA	LYS	714	37.301	15.389	26.425	1.00	43.70
MOTA	5583	CB	LYS	714	36.842	16.796	26.043	1.00	44.69
MOTA	5584	CG	LYS	714	38.001	17.746	25.836	1.00	47.92
MOTA	5585	CD	LYS	714	37.543	19.171	25.583	1.00	55.01
ATOM	5586	CE	LYS	714	38.733	20.077	25.238	1.00	59.44
MOTA	5587	NZ	LYS	714	39.773	20.132	26.320	1.00	60.10
ATOM	5591	C	LYS	714	36.127	14.557	26.940	1.00	43.94
ATOM	5592	0	LYS	714	35.843	14.551	28.140	1.00	44.20
ATOM	5593	N	GLU	715	35.477	13.819	26.046	1.00	43.29

						19	0				
AT			GLU	71-							
AT	-55	CB	GLU	715	34.	350	12.9	79 2	6.435	_	
AT	-55,		GLU	715	33.	464	12.6		5.225	1.00	42.29
ATO		CD	GLU	715	32.	913	13.9		1.522	1.00	44.91
ATO		OE1	~	715	32.	020	13.5		3.332	1.00	51.62
ATC		OE2	<b>~-</b>	715	32.	343	12.60			1.00	55.01
ATC	M 5601	C	A	715	30.	992	14.25		5.596	1.00	58.09
ATO		ō		715	34.8	306	11.66		.136	1.00	55.83
ATO	M 5603	N	<b>~</b>	715	33.9		10.82		.064	1.00	41.07
ATO		CA		716	36.1		11.47		.421	1.00	38.01
ATO		C		16	36.6		10.25		.182	1.00	41.11
MOTA	5607	0		16	36.5		9.05		. 770	1.00	39.69
ATOM				16	36.5	62			847	1.00	39.64
ATOM		N Cr	HIS 7	17	36.3	59	7.904	-	290	_	36.71
ATOM				17	36.2	15	9.335		554	_	41.95
ATOM			HIS 7	17	35.85		8.300	_	541	1.00	43.32
ATOM	5613	CG	HIS 71	۱7	35.81		8.918		183 j		43.38
ATOM	5614		HIS 71	.7	34.80		7.926		060 1		4.79
ATOM	5614 5616		HIS 71	7	36.91	_	7. <b>1</b> 52	21.	596 1		4.64
ATOM		CE1 F	IIS 71	7	36.58		7.625	· - · -	285 1		6 21
ATOM	~ ~ .		IIS 71	7	35.30		708	20.3	192 1		6.21
ATOM	F C C C		IS 71	7	37.48	_	.404	20.5	61 1		6.21 5.55
ATOM			IS 71	7	38.58		481	24.4			2.55
ATOM			RG 718	3	37.304	_	.031	24.3			3.90
ATOM	560.		RG 718		38.387	-	.169	24.2			5.45
ATOM			RG 718		38.500	_	.207	24.1			3.44
ATOM			RG 718		38.844	_	.361	25.4			2.68
ATOM		D AF			40.214		.165	26.65		-	00
ATOM		E AR	G 718		40.658	5 .	825	26.49	5 1.	_	.09
ATOM	5629 C	Z AR			40.521	6.	549	27.68	5 1.		.06
<b>-</b> ·	~	HI AR			39.940	7.	861	27.86	2 1.0		.51
T TO		H2 AR	G 718		11.024		608	26.93	1 1.0		.90
7.000	5636 C	AR		-	38.080		443	28.94	6 1.c		. 48
	5637 O	AR		,	16 022	4.	308	22.92	7 1.0		. 06
	2638 N	MET		-	6.911		007	22.650	1.0	_	.91
T COL	640 CA	MET		2	9.113		933	22.174			40
	641 CB	MET		3	8.928		79	21.004	1.0	- •	56
	642 CG	MET		4	0.219	2.9	64	20.181	1.0	-	82
	643 SD	MET		4	0.595	4.2	21 :	19.413	1.00		
	644 CE	MET			2.093	4.0	79 j	18.400	1.00		
	645 C	MET	719	7.	3.323	3.9	49 1	9.613	1.00		
	546 O	MET	719	30	3.460	1.6		1.432	1.00		
	547 N	ASP	720	20	822	1.2	16 2	2.516	1.00		4
	49 CA	ASP	720	3/	.635	1.0	752	0.582	1.00		6
ATOM 56	50 CB	ASP	720	3/	.090	-0.26	55 2	0.824		,	0
3	51 CG	ASP	720	36	.077	~0.66		9.733	1.00	45.5	
ATOM 56	52 OD1	ASP	720	34	.811	0.18		9.749	1.00	48.6	
ATOM 56		ASP	720	34	.678	1.08	2 20	0.612	1.00	53.0	
ATOM 56		ASP		33	. 943	-0.06		8.880	1.00	59.6	l
ATOM 56		ASP	720	38	177	-1.32		.823	1.00	50.58	3
ATOM 56		LYS	720	39.	235	-1.17	-	.199	1.00	43.64	1
ATOM 569		LYS	721	37.	876	-2.43		100	1.00	43.66	1
ATOM 565			721	38.	784	-3.569		-487	1.00	42.90	
ATOM 566		LYS	721	38.	278	-4.565		. 555	1.00	42.96	
ATOM 566		LYS	721	39.	000	-5.888		. 587	1.00	42.51	
-		LYS	721	38.		-6.805		. 570	1.00	47.68	
SSD/55145.	νΩ1					505	23.	628	1.00	51.61	
	- +/ 1										





ATOM	5662	CE	LYS	721	38.450	-8.246	23.163	1.00	54.96	
ATOM	5663	NZ	LYS	721	38.165	-9.190	24.282	1.00	59.67	
ATOM	5667	С	LYS	721	38.825	-4.215	20.182	1.00	43.05	
MOTA	5668	0	LYS	721	37.779	-4.577	19.625	1.00	46.08	
ATOM	5669	N	PRO	722	40.025	-4.348	19.601	1.00	43.22	
ATOM	5670	CD	PRO	722	41.337	-3.872	20.067	1.00	43.52	
ATOM	5671	CA	PRO	722	40.139	-4.968	18.275	1.00	41.04	
ATOM	5672	СВ	PRO	722	41.631	-4.856	17.965	1.00	40.87	
ATOM	5673	CG	PRO	722	42.074	-3.682	18.764	1.00	42.22	
ATOM	5674	C	PRO	722	39.726	-6.427	18.346	1.00	39.64	
ATOM	5675	0	PRO	722	39.730	-7.023	19.425	1.00	37.12	
MOTA	5676	N	SER	723	39.311	-6. <b>9</b> 82	17.212	1.00	40.36	
MOTA	5678	CA	SER	723	38.947	-8.389	17.158	1.00	41.41	
ATOM	5679	CB	SER	723	38.205	-8.707	15.865	1.00	38.26	
ATOM	5680	OG	SER	723	39.049	-8.520	14.749	1.00	43.87	
ATOM	5682	С	SER	723	40.294	-9.102	17.191	1.00	41.54	
ATOM	5683	0	SER	723	41.284	-8.575	16.703	1.00	40.90	
MOTA	5684	N	ASN	724	40.338	-10.300	17.750	1.00	44.89	
ATOM	5686	CA	ASN	724	41.598	-11.019	17.853	1.00	48.14	
ATOM	5687	СВ	ASN	724	42.256	-11.202	16.476	1.00	52.43	
MOTA	5688	CG	ASN	724	41.682	-12.374	15.715	1.00	57.29	
MOTA	5689	OD1	ASN	724	41.637	-13.492	16.225	1.00	61.96	
ATOM	5690	ND2	ASN	724	41.218	-12.125	14.500	1.00	60.91	
ATOM	5693	С	ASN	724	42.509	-10.255	18.811	1.00	48.17	
ATOM	5694	0	ASN	724	43.648	-9.918	18.495	1.00	49.88	
MOTA	5695	N	CYS	725	41.960	-9.935	19.973	1.00	47.12	
MOTA	5697	CA	CYS	725	42.686	-9.238	21.010	1.00	46.17	
ATOM	5698	CB	CYS	725	42.569	-7.717	20.862	1.00	44.83	
MOTA	5699	SG	CYS	725	43.459	-6.813	22.159	1.00	42.51	
MOTA	5700	С	CYS	725	42.017	-9.697	22.294	1.00	45.78	
MOTA	5701	0	CYS	725	40.803	-9.642	22.423	1.00	44.83	
MOTA	5702	N	THR	726	42.810	-10.224	23.212	1.00	45.63	
ATOM	5704	CA	THR	726	42.289	-10.711	24.482	1.00	45.47	
ATOM	5705	CB	THR	726	43.351	-11.545	25.217	1.00	45.93	
ATOM	5706	OG1	THR	726	44.307	-10.651	25.786	1.00	45.04	
MOTA	5708	CG2	THR	726	44.061	-12.495	24.233	1.00	42.99	
MOTA	5709	С	THR	726	41.858	-9.545	25.359	1.00	45.73	
ATOM	5710	0	THR	726	42.368	-8.445	25.216	1.00	46.91	
ATOM	5711	N	ASN	727	40.914		26.257	1.00	45.93	
ATOM	5713	CA	ASN	727	40.448	-8.736	27.141	1.00	47.85	
ATOM	5714	CB	ASN	727	39.300	-9.237	28.022	1.00	54.88	
MOTA	5715	CG	ASN	727	39.629	-10.544	28.731	1.00	65.11	
ATOM	5716	OD1	ASN	727	40.737	-10.734	29.229	1.00	70.58	
ATOM	5717	ND2	ASN	727	38.681	-11.472	28.735	1.00	69.68	
MOTA	5720	C	ASN	727	41.591	-8.212	27.999	1.00	44.18	
MOTA	5721	0	ASN	727	41.594	-7.047	28.390	1.00	41.35	
ATOM	5722	N	GLU	728	42.572	-9.073	28.260	1.00	42.82	
ATOM	5724	CA	GLU	728	43.725	-8.713	29.071	1.00	42.37	
ATOM	5725	CB	GLU	728	44.573	-9.952	29.379	1.00	43.09	
MOTA	5726	CG	GLU	728	45.806	-9.654	30.245	1.00	48.30	
MOTA	5727	CD	GLU	728	46.643	-10.889	30.568	1.00	50.11	
MOTA	5728	OE1	GLU	728	46.867	-11.732	29.668	1.00	47.98	
MOTA	5729	OE2	GLU	728	47.085	-11.010	31.733	1.00	51.69	
ATOM	5730	C	GLU	728	44.551	-7.652	28.356	1.00	39.57	





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	ATOM	5731	0	GĻU	728						
		5732	N	LEU	729	44.8	_	.605 2	8.933	1.00	30.50
1	ATOM	5734	CA	LEU	729	44.8			7.089	1.00	39.30
Į	MOTA	5735	CB	LEU		45.6			5.274	1.00	37.38
	MOTA	5736	CG	LEU	729	46.02	27 - 7.		1.935		36.74
	MOTA	5737	CD1	LEU	729	47.13	<sup>37</sup> -8.		5.001	1.00	35.39
A	TOM 5	5738	CD2		729	47.10	17 -9.		766	1.00	35.41
A		739	C	LEU	729	48.50			.174	1.00	35.69
		740	_	LEU	729	44.88				1.00	37.72
		~		LEU	729	45.46	7 -4.		.050	1.00	35.52
				TYR	730	43.56	5 -5.		. 941	1.00	33.96
				TYR	730	42.76			.000	1.00	32.90
	_	~		TYR	730	41.339	- • •		.812	1.00	32.41
				<b>TYR</b>	730	40.445			. 398	1.00	32.16
				ΓΥR	730	40.769			172	1.00	34.93
				TYR	730	39.962			203	1.00	32.49
				YR	730	39.282			994	1.00	32.80
		749 c	E2 1		730	38.465			931	1.00	33.45
AT			Z T		730	30.405	_				34.81
ATO		51 0	н т		730	38.814	~1.5				34.06
AT(		53 C			730	38.009	~0.4	65 24.			34.06
ATO		54 O			730	42.767	-3.7	88 27.			36.66
ATO		55 ท			731	42.837	-2.5	58 27.(			33.48
ATC	<b>.</b>	57 C			731	42.698	-4.46	66 28.2			34.94
ATO		58 CI		-	31	42.724	-3.75	55 29.5			35.29
ATO		59 CC				42.465	~4.70	9 30.6			38.38
ATO			• • • •		31	41.048	-5.26	4 30.7			12.01
ATO	M 576				31	39.785	-3.96				3.67
ATO	M 576		ME		31	39.828	-3.68				2.97
ATO		_		•	31	44.073	-3.04	9 29.6			1.83
ATON			ME		31	44.160	-1.95				4.52
ATOM	1 576		ME	-	32	45.118	-3.66				3.23
ATOM	1 576				32	46.445	-3.069				3.93
ATOM			ME			47.506	-3.995				6.26
ATOM			MET			48.935	-3.418		_		5.56
ATOM		_	MET		2	50.186	-4.522	_			5.26
ATOM			MET		2	50.480	-5.562			00 30	.46
ATOM		_	MET	73	2 .	46.369				00 26	.88
ATOM	9,,2		MET		2	46.827	-1.750			00 34	. 75
ATOM	5773		MET	73		45.741	-0.722 -1.774	28.87		00 35	.49
ATOM	5775		MET			45.571		27.21			. 63
ATOM	5776	CB	MET	733	•	44.787	-0.566	26.41		0 32	. 79
MOTA	5777		MET	733		45.544	-0.853	25.130	1.0	0 33	.16
	5778	SD	MET	733		44.421	-1.601	24.047	1.0	0 32	. 32
ATOM	5779	CE	MET	733		15.155	-1.990	22.670	1.0		66
ATOM	5780	C	MET	733		14.789	-3.496	22.068		0 29.	
ATOM	5781	0	MET	733			0.452	27.229	1.0		
ATOM	5782	N	ARG	734	•	15.176	1.619	27.318			
ATOM	5784	CA	ARG	734	-	3.679	0.018	27.818		_	
ATOM	5785	CB	ARG	734		2.854	0.913	28.621	1.00		
ATOM	5786	CG	ARG			1.586	0.197	29.095	1.00		
ATOM	5787	CD		734		0.726	-0.335	27.950			
ATOM	5788	NE	ARG	734		0.256	0.783	27.043	1.00	• .	
ATOM	5790	CZ	ARG	734		9.416	1.745	27.750	1.00	-	
ATOM	5791		ARG	734	3	8.092	1.661		1.00		
ATOM	5794	NH1	ARG	734		7.439	0.660	27.844	1.00		
	J, J3	NH2	ARG	734		7.420	2.571	27.268	1.00		
SSSD/55	145						5/1	28.530	1.00	44.6	55
	13. VU1										

ATOM	<b>5</b> 797	С	ARG	734	43.660	1.458	29.793	1.00	32.12
MOTA	5798	0	ARG	734	43.492	2.610	30.180	1.00	35.37
MOTA	5799	N	ASP	735	44.566	0.646	30.327	1.00	33.75
MOTA	5801	CA	ASP	735	45.438	1.076	31.433	1.00	36.72
ATOM	5802	CB	ASP	735	46.379	-0.055	31.857	1.00	42.71
ATOM	5803	CG	ASP	735	45.722	-1.052	32.774	1.00	47.31
ATOM	5804	OD1	ASP	735	46.124	-2.241	32.720	1.00	50.99
MOTA	5805	OD2	ASP	735	44.824	-0.646	33.552	1.00	48.45
MOTA	5806	С	ASP	735	46.291	2.251	30.972	1.00	34.25
MOTA	5807	0	ASP	735	46.376	3.286	31.648	1.00	34.31
ATOM	5808	N	CYS	736	46.927	2.064	29.816	1.00	31.85
MOTA	5810	CA	CYS	736	47.780	3.077	29.204	1.00	29.93
ATOM	5811	CB	CYS	736	48.413	2.545	27.921	1.00	24.97
ATOM	5812	SG	CYS	736	49.504	1.159	28.180	1.00	31.35
ATOM	5813	С	CYS	736	46.994	4.325	28.885	1.00	31.62
ATOM	5814	0	CYS	736	47.562	5.416	28.823	1.00	30.73
ATOM	5815	N	TRP	737	45.680	4.174	28.711	1.00	35.03
ATOM	5817	CA	TRP	737	44.812	5.308	28.395	1.00	36.35
ATOM	5818	CB	TRP	737	43.808	4.927	27.297	1.00	36.43
ATOM ATOM	5819	CG	TRP	737	44.451	4.487	26.010	1.00	34.34
MOTA	5820	CD2	TRP	737	43.914	3.565	25.052	1.00	34.81
ATOM	5821 5822	CE2 CE3	TRP	737	44.852	3.461	23.999	1.00	33.92
ATOM	5823	CD1	TRP TRP	737 737	42.730	2.816	24.980	1.00	33.06
ATOM	5824	NE1	TRP	737	45.659 45.907	4.890 4.279	25.514	1.00	35.19
ATOM	5826	CZ2	TRP	737	44.644	2.633	24.309 22.886	1.00	35.00
ATOM	5827	CZ3	TRP	737	42.527	1.991	23.876	1.00 1.00	33.45
MOTA	5828	CH2	TRP	737	43.480	1.909	22.844	1.00	32.92 30.45
ATOM	5829	C	TRP	737	44.080	5.895	29.609	1.00	37.23
ATOM	5830	0	TRP	737	43.047	6.551	29.474	1.00	37.44
ATOM	5831	N	HIS	738	44.624	5.681	30.798	1.00	41.45
MOTA	5833	CA	HIS	738	44.006	6.208	32.008	1.00	41.52
MOTA	5834	CB	HIS	738	44.675	5.635	33.258	1.00	41.23
MOTA	5835	CG	HIS	738	43.925	5.924	34.522	1.00	43.31
MOTA	5836	CD2	HIS	738	43.618	7.096	35.126	1.00	41.58
MOTA	5837	ND1	HIS	738	43.338	4.935	35.279	1.00	44.22
MOTA	5839	CE1	HIS	738	42.693	5.487	36.294	1.00	46.62
ATOM	5840	NE2	HIS	738	42.848	6.798	36.223	1.00	43.99
ATOM	5842	С	HIS	738	44.118	7.726	32.015	1.00	41.75
ATOM	5843	0	HIS	738	45.179	8.268	31.731	1.00	40.84
MOTA	5844	N	ALA	739	43.025	8.405	32.352	1.00	42.47
ATOM	5846	CA	ALA	739	43.004	9.873	32.398	1.00	44.58
MOTA	5847	CB	ALA	739	41.629	10.361	32.825	1.00	48.19
MOTA	5848	С	ALA	739	44.081	10.467	33.317	1.00	45.12
MOTA	5849	0	ALA	739	44.653	11.510	33.020	1.00	45.66
MOTA	5850	N	VAL	740	44.262	9.852	34.481	1.00	46.64
MOTA	5852	CA	VAL	740	45.278	10.273	35.453	1.00	46.78
MOTA	<b>585</b> 3	CB	VAL	740	44.867	9.893	36.888	1.00	47.74
ATOM	5854	CG1	VAL	740	45.919	10.372	37.890	1.00	49.35
MOTA	5855	CG2	VAL	740	43.515	10.495	37.211	1.00	47.89
ATOM	5856	C	VAL	740	46.601	9.573	35.121	1.00	45.24
MOTA	5857	0	VAL	740	46.754	8.362	35.347	1.00	45.01
ATOM	5858	N	PRO	741	47.588	10.335	34.637	1.00	43.46
MOTA	5859	CD	PRO	741	47.536	11.794	34.437	1.00	43.51

								_				
A	TOM	5860	CA	PRO	7/1							
A	TOM 5	5861	CB	PRO	741 741	48.9			804 34	. 266	1.00	16.22
		862	CG	PRO	741	=- • •		11.0	070 33	942	1.00	
A'	TOM 5	863	С	PRO		48.63		12.0		426	1.00	
		864	0	PRO	741	49.58		8.9		328	1.00	
A	rom 5	865		SER	741	50.24		7.9		994	1.00	
A?	rom 5	867	~-	SER	742	49.39		9.2		601		45.12
AT	OM 5	~			742	49.99	4	8.5		703	1.00	48.78
AT					742	49.84	5	9.3				48.76
AT	'OM 5		~		742	48.48		9.4			1.00	51.11
AT	OM 58				742	49.37		7.1			1.00	53.50
AT	OM 58				742	49.93		6.28	-		1.00	47.77
ATO		. ~ _			743	48.199		6.96			1.00	47.31
ATO				<b></b> .	743	47.51		5.68			1.00	47.57
ATO		~			743	46.004		5.91			1.00	47.14
ATO			-	_	43	45.438		5.44			1.00	50.16
ATC		~			43	46.239		5.96			1.00	54.69
ATO					43	46.898		5.19	· · · · · · · · · · · · · · · · · · ·		1.00	57.62
ATO					43	46.202		7.27			1.00	59.09
ATO		-		LN 7	43	47.816		4.77	· –		00	59.45
ATO		_	٠.		43	47.365		3.62			00	44.41
ATO		_		RG 74	44	48.515		5.30			.00	44.39
ATO				2G 74	14	48.902		1.50e			.00	42.87
ATON		_		G 74	4	49.350					.00	41.45
ATOM				G 74	4	48.316		397				37.34
ATOM				G 74	4	48.854		.380				32.30
ATOM		_		G 74	4	47.921		.207			.00	31.37
ATOM						48.271		.276			.00	36.76
ATOM		_		G 74	4	49.553		.492				39.88
			2 ARG			47.330		.813	30.39		00	39.94
ATOM			ARC	74	4	50.068		.404	30.32			39.12
ATOM			ARG			50.813		.616	34.47			11.40
ATOM	5902		PRO			50.203		945	35.409	5 1.		2.84
ATOM	5903		PRO			49.345		441	33.849			0.11
ATOM	5904		PRO			51.332		739	32.876	1.		9.91
ATOM	5905	CB	PRO			51.019		607	34.266	1.		8.58
ATOM	5906	CG	PRO			50.250		261	33.605	1.0		7.46
ATOM	5907	C	PRO	745				645	32.377	1.0		7.41
ATOM	5908	0	PRO	745		52.640		202	33.750	1.0		7.73
ATOM	5909	N	THR	746		52.634		027	32.835	1.0	-	7.71
ATOM	5911	CA	THR	746		53.753		B43	34.373	1.0		5.90
ATOM	5912	CB	THR	746		55.050 56.005		328	33.913	1.0	_	1.77
ATOM	5913	OG1	THR	746		56.085	2.3	380	35.075	1.0		. 85
MOTA	5915	CG2	THR	746		56.296	1.0	)59	35.602	1.0		. 92
ATOM	5916	С	THR	746		55.605	3.3		36.177	1.0	-	.17
MOTA	5917	0	THR	746		55.544	1.3		32.870	1.0		.69
ATOM	5918	N	PHE	747		55.026	0.2		32.795	1.00		
ATOM	5920	CA	PHE			56.538	1.7	80	32.066	1.00		. 56
ATOM	5921	CB	PHE	747		57.093	0.7	82	31.083	1.00		. 04
MOTA	5922	CG	PHE	747		8.121	1.4		30.193	1.00		. 74
ATOM	5923	CD1		747		7.504	2.2		29.096			
	5924	CD2	PHE	747		6.772	1.6		28.092	1.00		
	5925	CE1	PHE	747	5	7.609	3.66		29.091	1.00		
	5926		PHE	747	5	6.170	2.40		27.100	1.00		
<b>3</b>	5927	CE2	PHE	747	5	7.001	4.41		28.091	1.00		
	-261	CZ	PHE	747	5	6.276	3.77		28.091	1.00		
SSSD/551	45. v01								103	1.00	25.	73

ATOM	5928	С	PHE	747	57.714	-0.413	31.782	1.00	31.92
ATOM	5929	0	PHE	747	57.727	-1.514	31.243	1.00	32.46
MOTA	5930	N	LYS	748	58.233	-0.199	32.986	1.00	33.47
ATOM	5932	CA	LYS	748	58.816	-1.302	33.733	1.00	35.57
MOTA	5933	CB	LYS	748	59.468	-0.800	35.026	1.00	39.42
ATOM	5934	CG	LYS	748	60.083	-1.923	35.861	1.00	46.49
MOTA	5935	CD	LYS	748	60.817	-1.407	37.103	1.00	50.69
MOTA	5936	CE	LYS	748	61.253	-2.574	37.999	1.00	52.57
ATOM	5937	NZ	LYS	748	62.072	-2.129	39.155	1.00	56.45
ATOM	5941	C	LYS	748	57.700	-2.318	34.028	1.00	35.58
ATOM	5942	0	LYS	748	57.898	-3.526	33.871	1.00	34.72
MOTA	5943	N	GLN	749	56.522	-1.818	34.411	1.00	35.59
MOTA	5945	CA	GLN	749	55.369	-2.684	34.692	1.00	38.20
ATOM	5946	CB	GLN	749	54.154	-1.872	35.162	1.00	42.73
ATOM	5947	CG	GLN	749	54.264	-1.171	36.499	1.00	49.30
ATOM	5948	CD	GLN	749	53.060	-0.282	36.761	1.00	53.13
MOTA	5949	OE1	GLN	749	53.194	0.915	37.023	1.00	52.71
ATOM	5950	NE2	GLN	749	51.873	-0.856	36.644	1.00	58.54
ATOM	5953	C	GLN	749	54.954	-3.392	33.409	1.00	36.16
ATOM	5954	0	GLN	749	54.745	-4.605	33.393	1.00	36.67
ATOM	5955	N	LEU	750	54.801	-2.609	32.342	1.00	35.83
MOTA	5957	CA	LEU	750	54.381	-3.117	31.037	1.00	34.49
ATOM	5958	CB	LEU	750	54.324	-1.988	30.004	1.00	32.49
MOTA	5959	CG	LEU	750	53.206	-0.958	30.188	1.00	31.94
MOTA	5960	CD1	LEU	750	53.411	0.230	29.267	1.00	30.45
MOTA	5961	CD2	LEU	750	51.859	-1.610	29. <b>9</b> 33	1.00	29.30
ATOM	5962	С	LEU	750	55.294	-4.214	30.559	1.00	33.87
ATOM	5963	0	LEU	750	54.828	-5.208	30.027	1.00	34.72
MOTA	5964	N	VAL	751	56.598	-4.038	30.759	1.00	36.12
ATOM	5966	CA	VAL	751	57.585	-5.045	30.363	1.00	34.50
ATOM	5967	CB	VAL	751	59.054	-4.532	30.559	1.00	31.96
MOTA	5968	CG1	VAL	751	60.052	-5.646	30.308	1.00	30.24
ATOM	5969	CG2	VAL	751	59.342	-3.386	29.604	1.00	28.02
MOTA	5970	C	VAL	751	57.349	-6.321	31.182	1.00	36.11
ATOM	5971	0	VAL	751	57.333	-7.422	30.638	1.00	36.45
ATOM	5972	N	GLU	752	57.107	-6.1 <b>6</b> 5	32.479	1.00	37.83
ATOM	5974	CA	GLU	752	56.869	-7.326	33.331	1.00	41.47
ATOM	5975	CB	GLU	752	56.800	-6.910	34.804	1.00	43.03
ATOM	5976	CG	GLU	752	58.122	-6.305	35.263	1.00	52.52
ATOM	5977	CD	GLU	752	58.251	-6.176	36.761	1.00	57.18
MOTA	5978	OE1	GLU	752	58.600	-5.068	37.233	1.00	58.11
ATOM	5 <b>9</b> 79	OE2	GLU	752	58.032	-7.191	37.461	1.00	61.59
ATOM	5980	С	GLU	752	55.623	-8.097	32.890	1.00	40.16
ATOM	5981	0	GLU	752	55.689	-9.308	32.642	1.00	39.75
ATOM	5982	N	ASP	753	54.524	-7.376	32.696	1.00	40.06
MOTA	5984	CA	ASP	753	53.275	-7.982	32.264	1.00	39.73
ATOM	5985	CB	ASP	753	52.157	-6.947	32.247	1.00	41.00
MOTA	5986	CG	ASP	753	51.668	-6.591	33.640	1.00	45.17
ATOM	5987	OD1	ASP	753	51.753	-7.468	34.543	1.00	49.78
MOTA	5988	OD2	ASP	753	51.210	-5.439	33.829	1.00	45.51
MOTA	5989	C	ASP	753	53.396	-8.595	30.890	1.00	39.64
MOTA	5990	0	ASP	753	52.955	-9.720	30.674	1.00	41.84
ATOM	5991	N	LEU	754	53.998	-7.861	29.960	1.00	37.75
MOTA	5993	CA	LEU	754	54.161	-8.358	28.603	1.00	38.16

A'	TOM 5	994	CD	<b>-</b>								
		995		LEU	754			-7.	261 27	7.664	1 /	20 25
		996		LEU	754	-5.5		-6.		7.307		
	-			LEU	754			-5.0		.590		
			_	LEU	754	<b>-</b>		-6.9		.465		
			_	LEU	754	-0.0		-9.5		.571	1.0	
				LEU	754	54.9	05	-10.4		.740	1.0	
				ASP	755	56.0	14	-9.6		.502	1.0	55
AT				ASP	755	56.93	30	-10.7		. 594	1.0	
AT		_		SP	755	57.95	56	-10.4		.696	1.0	
AT				SP	755	59.12	28	-11.4		652	1.0	
ATO				SP	755	59.75	59	-11.6		711	1.0	03
ATO				SP.	755	59.43	32	-11.9		565	1.00	
ATO				SP	755	56.08		-11.9		947	1.00	
ATC		_		SP	755	56.15		-12.99			1.00	
ATC			_	RG	756	55.23		-11.77		289	1.00	_
ATO			_	RG	756	54.34		-12.81		955	1.00	
ATO		_		₹G	756	53.57		-12.31		437	1.00	,
ATO		_			756	52.43		-13.21			1.00	
ATO		_		₹G	756	51.79		-12.63			1.00	_
ATO		_			756	51.353		-11.24			1.00	
ATO				G	756	50.295		-10.89			1.00	
ATO					756	49.549		-11.81			1.00	48.17
ATON					756	49.998		-9.60	-		1.00	46.64
ATOM			AR		756	53.362		-13.27			1.00	48.92
ATON		_	AR		756	53.247		-14.469	-		1.00	40.19
ATOM			IL		757	52.688		-12.327			1.00	42.24
ATOM					57	51.706		-12.649			1.00	38.18
ATOM					57	50.952		11.382			1.00	38.40
ATOM					57	49.952		11.758			1.00	36.55
ATOM					57	50.216		10.726			1.00	34.67
ATOM					57	49.554		-9.423			1.00	34.65
ATOM			ILE		57	52.301	_	13.400			L.00	36.49
ATOM		_	ILE		57	51.709		14.360			.00	39.19
ATOM	6033		VAL		58	53.492		12.996	27.06		00	39.66
ATOM	6038		VAL		58	54.161		13.645	25.93		00	42.36
ATOM		СВ	VAL		8	55.582		13.052	25.68		.00	43.15
ATOM	6039	CG1		75	8	56.308		13.855	24.62		.00	41.72
ATOM	6040 6041	CG2		75		55.491		L1.619	25.22		.00	41.57
ATOM	6041	C	VAL	75		54.299		15.133	26.23		.00	40.06
ATOM	6043	0	VAL	75	-	54.045		5.971	25.36		.00	47.11
ATOM	6045	N	ALA	75		54.695		5.446	27.46	-	.00	48.62
ATOM	6046	CA	ALA	75		54.879		6.820	27.90		.00	49.64
ATOM		CB	ALA	75	9	55.423		6.830	29.31			51.35
ATOM	6047	C	ALA	75	9	53.568		7.598				50.11
ATOM	6048	0	ALA	75	9	53.520		8.717	27.850			54.72
ATOM	6049	N	LEU	76	כ	52.496	- 1	6.983	27.348			58.64
	6051	CA	LEU	760	)	51.194		7.628	28.329			54.84
ATOM ATOM	6052	CB	LEU	760	)	50.330		7.028	28.343			55.87
ATOM	6053	CG	LEU	760	)	50.875		7.165	29.459			56.85
	6054	CD1	LEU	760	)	49.991		5.392	30.885			56.80
ATOM	6055	CD2	LEU	760	)	50.959		3.631	31.849		_	56.78
ATOM	6056	C	LEU	760				7.546	31.289		-	57.78
ATOM	6057	0	LEU	760				7.859	27.013	1.0		7.36
ATOM	6058	N	THR	761				.859 .134	26.944	1.0		7.65
SSSD/55	145 201						/	. 134	25.956	1.0	00 5	8.71

ATOM	6060	CA	THR	761	50.541	-17.025	24.630	1.00	59.04	
MOTA	6061	CB	THR	761	50.839	-15.657	23.971	1.00	56.72	
ATOM	6062	OG1	THR	761	50.287	-14.610	24.775	1.00	56.53	
ATOM	6064	CG2	THR	761	50.213	-15.584	22.590	1.00	53.81	
MOTA	6065	С	THR	761	51.049	-18.138	23.721	1.00	60.44	
MOTA	6066	0	THR	761	<b>52.25</b> 5	-18.295	23.530	1.00	61.40	
MOTA	6067	SG	CYS	1603	18.474	-8.976	20.202	0.50	37.82	PRT2
ATOM	6068	CG	MET	534	69.311	12.109	23.281	0.50	36.25	PRT2
MOTA	6069	SD	MET	534	69.286	12.958	24.867	0.50	42.66	PRT2
ATOM	6070	CE	MET	534	70.539	12.083	25.804	0.50	43.27	PRT2
ATOM	6071	SG	CYS	603	56.046	-7.949	16.446	0.50	36.47	PRT2
MOTA	2676	OH2	TIP3	1	71.794	25.061	2.660	1.00	24.53	
MOTA	2679	OH2	TIP3	2	39.750	3.992	15.898	1.00	39.62	
ATOM	2682	OH2	TIP3	3	83.809	19.717	10.596	1.00	28.26	
MOTA	2685	OH2	TIP3	4	83.630	20.056	7.685	1.00	26.19	
ATOM	2688	OH2	TIP3	5	75.073	16.616	6.785	1.00	26.48	
MOTA	2691	OH2	TIP3	6	86.549	19.594	9.502	1.00	33.65	
MOTA	2694	OH2	TIP3	7	51.913	11.060	24.263	1.00	35.55	
MOTA	2697	OH2	TIP3	8	55.093	9.421	22.524	1.00	26.63	
ATOM	2700	OH2	TIP3	9	57.161	4.614	32.443	1.00	29.69	
MOTA	2703	OH2	TIP3	10	52.169	4.735	13.281	1.00	22.61	
MOTA	2706	OH2	TIP3	11	41.110	5.543	22.764	1.00	41.60	
MOTA	2709	OH2	TIP3	12	45.145	8.857	21.555	1.00	36.99	
ATOM	2712	OH2	TIP3	13	64.465	-2.607	28.883	1.00	30.17	
ATOM	2715	OH2	TIP3	14	76.944	13.287	23.954	1.00	32.94	
MOTA	2718	OH2	TIP3	15	79.062	17.048	18.200	1.00	51.65	
MOTA	2721	OH2	TIP3	16	83.066	11.657	15.958	1.00	25.12	
ATOM	2724	OH2	TIP3	17	13.957	-9.951	0.095	1.00	26.02	
MOTA	2727	OH2	TIP3	18	38.359	-0.001	5.000	1.00	37.43	
ATOM	2730	OH2	TIP3	19	5.442	2.705	19.077	1.00	29.46	
MOTA	2733	OH2		20	27.008	6.166	4.885	1.00	25.05	
ATOM	2736	OH2	TIP3		34.242	-1.725	16.911	1.00	52.12	
MOTA	2739	OH2	TIP3		20.167	2.428	27.681	1.00	42.69	
ATOM	2742	OH2		23	50.794	-11.834	38.045	1.00	60.16	
ATOM	2745	OH2		24	17.261	-5.993	-1.757	1.00	25.88	
ATOM	2748	OH2	TIP3		27.516	7.803	15.070	1.00	39.33	
ATOM	2751	OH2	TIP3		31.574	0.146	6.684	1.00	35.78	
MOTA	2754	OH2	TIP3		27.119	-12.972	27.844	1.00	43.66	
MOTA	2757	OH2	TIP3		28.439	-17.074	13.203	1.00	36.44	
MOTA	2760	OH2	TIP3		88.706	14.393	7.969	1.00	32.49	
MOTA	2763	OH2	TIP3		-2.338	-3.424	11.295	1.00	49.20	
ATOM	2766	OH2	TIP3		35.086	-4.130	18.836	1.00	37.83	
MOTA	2769	OH2	TIP3		80.455	17.922	9.507	1.00	23.69	
ATOM	2772	OH2		33	5.538	3.619	10.835	1.00	29.13	
MOTA	2775	OH2	TIP3		-10.685	5.290	11.288	1.00	24.40	
MOTA	2778	OH2	TIP3		29.210	-8.799	20.241	1.00	46.52	
MOTA	2781	OH2	TIP3		6.195	3.150	13.803	1.00	31.39	
MOTA	2784	OH2	TIP3		31.898	2.830	0.154	1.00	40.17	
ATOM	2787	OH2	TIP3		19.915	2.023	-3.939	1.00	31.34	
MOTA	2790	OH2	TIP3		62.242	2.604	32.859	1.00	39.67	
MOTA	2793	OH2	TIP3		21.231	-7.063	-3.900	1.00	23.55	
MOTA	2796	OH2	TIP3		-15.809	8.838	22.610	1.00	36.02	
MOTA	2799	OH2	TIP3		40.120	2.154	8.433	1.00	60.62	
ATOM	2802	OH2	TIP3	43	19.583	11.128	-0.045	1.00	37.85	



ATO			2 TIP	3 44	67.05	6 9.03	17.700		
ATO		08 OH:	2 TIP	3 45	87.77				
ATC			2 TIP	3 46	74.58				
ATC		14 OH:	TIP:	3 47	29.36				
ATO			P TIP:	3 48	66.48				
ATO			TIP:	3 49	85.00				
ATO			TIPS	50	-4.57		_		
ATO			TIPE	51	19.49		_		
ATO			TIPS	52	67.49			1.00	
ATO			TIP3	53	34.79				
ATO			TIP3	54	34.78			1.00	40.16
ATO			TIP3	55	59.972		13.756 27.870	1.00	39.46
ATO			TIP3	56	-7.139		6.345	1.00	31.56
ATON			TIP3	57	54.998		25.360	1.00	42.00
ATON			TIP3	58	68.697		16.740	1.00	42.05
ATOM			TIP3	59	73.750		19.041	1.00	46.12
ATOM			TIP3	60	3.431			1.00	32.26
ATOM			TIP3	61	37.904		-8.218 5.612	1.00	31.22
ATOM			TIP3	62	29.982		-1.303	1.00	33.72
ATOM			TIP3	63	66.918		8.678	1.00	39.11
ATOM			TIP3	64	49.117		12.227	1.00	34.68
ATOM	-000		TIP3	65	41.246	3.987	29.033	1.00	34.31
ATOM			TIP3	<b>6</b> 6	10.755	-12.957	1.167	1.00	34.55
ATOM			TIP3	67	-1.184	-4.327	21.439	1.00	42.14
ATOM	,,		TIP3	68	30.349	16.267	13.265	1.00	37.90
ATOM	2880			69	8.111	4.362	3.445	1.00	55.23
ATOM ATOM	2883	OH2	TIP3	70	73.131	18.780	22.628	1.00	23.88
ATOM	2886	OH2	TIP3	71	-7.949	-3.409	24.953	1.00	40.20
ATOM	2889	OH2	TIP3	72	66.379	-4.621	28.423	1.00	35.49 45.46
ATOM	2892	OH2		73	21.506	-20.711	4.815	1.00	52.46
ATOM	2895 2898	OH2	_	74	59.539	-6.865	4.928	1.00	48.87
ATOM	2901	OH2		75	16.565	-13.297	-3.008	1.00	51.80
ATOM	2904	OH2 OH2		76	-15.235	7.385	4.428	1.00	29.13
ATOM	2907	OH2		77	32.926	2.785	13.213	1.00	37.62
ATOM	2910	OH2		78	0.246	-2.768	10.996	1.00	28.25
ATOM	2913	OH2		79	17.495	2.354	5.447	1.00	23.63
ATOM	2916	OH2		80	6.336	2.434	21.950	1.00	29.56
ATOM	2919	OH2		31 32	27.374	3.628	6.163	1.00	34.06
ATOM	2922	OH2	TIP3 6		-8.708	6.263	9.522	1.00	30.34
ATOM	2925		TIP3 6		1.500	-1.935		1.00	27.61
ATOM	2928			35	-4.825	-3.133		1.00	33.50
ATOM	2931		TIP3 8		17.513	2.839	1.966		24.27
ATOM	2934		TIP3 8		20.298	3.414		1.00	26.15
ATOM	2937			8	0.488				25.95
ATOM	2940			9	19.939	-6.185			19.14
ATOM	2943		-	0	10.670	-15.654	6.839	_	33.36
ATOM	2946		TIP3 9		4.107		11.805	_	33.92
ATOM	2949		TIP3 9		6.238	0.927			23.31
ATOM	2952		TIP3 9		-13.563	1.438	5.472		27.86
ATOM	2955		TIP3 9		15.707	-7.454			26.69
ATOM	2958		rips 9		-1.856	-5.393			39.91
MOTA	2961		TIP3 9		12.654 69.774	4.928		.00 3	31.32
MOTA	2964		TIP3 9		24.636	27.363	_		35.86
				•	47.030	-13.192	0.040 1	.00 4	18.53

ATOM	2967	OH2	TIP3	98	60.453	-4.625	33.829	1.00	31.97
MOTA	2970	OH2	TIP3	99	10.513	5.719	3.487	1.00	38.90
ATOM	2973	OH2	TIP3	100	-9.499	-4.011	4.342	1.00	30.61
ATOM	2976	OH2	TIP3	101	73.056	-1.608	10.514	1.00	36.08
ATOM	2979	OH2	TIP3	102	-3.152	5.709	30.608	1.00	29.38
ATOM	2982	OH2	TIP3	103	36.630	0.702	11.792	1.00	47.80
ATOM	2985	OH2	TIP3	104	21.475	6.325	16.924	1.00	24.03
ATOM	2988	OH2	TIP3	105	31.272	0.656	19.432	1.00	53.74
MOTA	2991	OH2	TIP3	106	5.620	-8.417	22.266	1.00	51. <b>9</b> 0
ATOM	2994	OH2	TIP3	107	-13.144	8.294	17.464	1.00	35.23
ATOM	2 <b>9</b> 97	OH2	TIP3	108	26.680	-10.556	-1.042	1.00	27.83
ATOM	3000	OH2	TIP3	109	24.149	1.846	18.172	1.00	30.90
MOTA	3003	OH2	TIP3	110	-1.943	12.643	3.558	1.00	33.82
ATOM	3006	OH2	TIP3	111	59.560	13.617	33.196	1.00	54.79
ATOM	3009	OH2	TIP3	112	4.351	-10.740	1.991	1.00	37.96
MOTA	3012	OH2	TIP3	113	8.396	2.913	0.958	1.00	29.64
ATOM	3015	OH2	TIP3		75.905	1.753	25.812	1.00	38.73
ATOM	3018	OH2	TIP3	115	48.783	15.535	14.189	1.00	35.24
ATOM	3021	OH2	TIP3	116	2.419	-11.312	9.146	1.00	32.85
ATOM	3024	OH2	TIP3	117	83.014	26.360	12.964	1.00	41.83
MOTA	3027	OH2	TIP3	118	8.761	-6.579	~3.252	1.00	42.78
ATOM	3030	OH2	TIP3	119	-8.417	4.493	4.305	1.00	28.32
ATOM	3033	OH2	TIP3	120	7.908	-13.690	8.639	1.00	33.73
ATOM	3036	OH2	TIP3	121	51.437	6.329	10.373	1.00	31.72
ATOM	3039	OH2	TIP3	122	20.660	3.686	15.591	1.00	32.37
ATOM	3042	OH2	TIP3	123	73.039	3.790	20.450	1.00	35.80
ATOM	3045	OH2	TIP3	124	5.155	-11.467	22.590	1.00	45.12
ATOM ATOM	3048	OH2		125	34.172	2.412	16.576	1.00	41.90
ATOM	3051 3054	OH2		126	9.597	-11.905	7.083	1.00	24.83
ATOM	3054	OH2 OH2		127	8.276	3.860	-1.622	1.00	35.46
ATOM	3060	OH2		128 129	66.282	5.755	12.352	1.00	35.43
ATOM	3063	OH2		130	7.377	6.932	2.982	1.00	40.68
ATOM	3066	OH2		131	35.832 44.781	-1.778	0.201	1.00	34.99
ATOM	3069	OH2		132	27.790	10.362 -12.638	11.064	1.00	42.31
ATOM	3072	OH2		133	45.221	11.540	18.958 21.428	1.00	58.71
ATOM	3075	OH2		134	57.560	-10.846	14.099	1.00	36.75
MOTA	3078	OH2		135	-3.354	15.001	16.515	1.00	52.90 37.81
MOTA	3081	OH2	TIP3		85.717	11.251	9.062	1.00	35.18
ATOM	3084	OH2	TIP3		12.951	-2.469	2.075	1.00	22.07
ATOM	3087	OH2	TIP3		75.645	3.486	20.527	1.00	38.01
ATOM	3090	OH2	TIP3		13.237	7.412	-2.649	1.00	33.50
ATOM	3093	OH2	TIP3		11.262	-9.970	0.974	1.00	26.14
ATOM	3096	OH2	TIP3		59.480	10.772	14.098	1.00	52.08
ATOM	3099	OH2	TIP3	142	13.869	-16.121	3.919	1.00	40.06
ATOM	3102	OH2	TIP3		-6.407	-3.413	16.641	1.00	44.38
ATOM	3105	OH2	TIP3		25.667	-12.645	3.411	1.00	48.28
ATOM	3108	OH2	TIP3		-16.282	10.641	6.423	1.00	40.94
ATOM	3111	ОН2	TIP3		86.637	12.861	7.008	1.00	39.45
ATOM	3114	OH2	TIP3		32.082	-4.569	1.892	1.00	27.35
MOTA	3117	OH2	TIP3		44.809	7.627	11.670	1.00	35.65
MOTA	3120	OH2	TIP3		80.693	12.459	16.523	1.00	37.21
MOTA	3123	OH2	TIP3		2.941	-7.118	-1.805	1.00	38.43
ATOM	3126	OH2	TIP3	151	31.794	-6.086	20.704	1.00	42.80



ATO		_	Н2 Т	IP3	152	74.77	ი -ა ი	02		
ATO	_	32 OI	Н2 Т	IP3	153					-
ATO		35 OF	H2 T	IP3	154	71.61	-			35.61
ATO		38 OI	H2 T	IP3	155	68.113				
ATC		11 OF	12 T	<b>I</b> P3	156	0.042				
ATC			12 T)	[P3	157	68.020				33.08
ATO			_	P3	158	3.795				
ATO		OH OH	[2 T]	P3	159	52.106				
ATO		3 OH	[2 TI		160	6.414				
ATO		6 OH	2 TI	<b>P</b> 3	161	-10.282	_		_	37.07
ATO			2 TI	P3	162	76.410		_		38.48
ATO		2 OH	2 TI	<b>P</b> 3	163	9.910	1.68 -12.04	_	_	42.87
ATO		5 OH:			164	33.983			_	32.79
ATO		8 OH:			165	2.330	14.21			37.35
ATO		1 OH			166	29.701	-7.95		_	44.25
ATON		4 OH2	2 TI		167	32.494	1.78			39.86
ATOM		7 OH2	2 TII		168	42.107	-17.31		-,,,	38.46
ATOM		О ОН 2	? TI		169	87.822	17.932	_	_	44.83
ATOM		OH2	TI		170	70.261	10.537			54.30
ATOM		OH2	TIE		71	77.519	-4.143			44.75
ATOM			TIF		.72	-0.921	5.882	_		42.67
ATOM			TIP	3 1	.73	34.213	-8.166			45.91
ATOM			TIP		74	-9.647	15.329			40.10
ATOM			TIP	3 1	75	11.619	7.73 <u>1</u> 5.799			35.63
ATOM			TIP	3 1	76	-8.709	13.964	•		36.36
ATOM			TIP	3 1	77	31.770	3.376			51.97
ATOM	,	OH2	TIP	3 1	78	-8.494	9.789	18.354	1.00	46.26
ATOM	3210	OH2	TIP	3 1	79	-1.234	-6.253	24.269	1.00	50.98
ATOM	3213	OH2	TIP	3 1	80	80.252	0.887	15.622	1.00	38.47
ATOM	3216	OH2	TIP	3 1	81	67.248	20.272	15.691	1.00	39.48
ATOM	3219	OH2	TIP:	3 1	B2	-0.566	4.367	-1.555	1.00	48.22
ATOM	3222	OH2	TIP	3 10	33	0.120	6.523	1.362	1.00	39.84
ATOM	3225	OH2	TIPE	3 18	34	-1.496	8.789	2.615	1.00	33.11
ATOM	3228	OH2	TIP3	18	35	-5.143	9.130	1.237 2.236	1.00	41.03
ATOM	3231	OH2	TIP3	18	36	-7.275	10.106	3.833	1.00	40.47
ATOM	3234	OH2	TIP3	18	37	2.717	7.275	0.769		40.55
ATOM ATOM	3237	OH2	TIP3		8	5.176	10.645	8.459		44.67
ATOM	3240	OH2	TIP3		9	63.822	12.690	22.883		34.48
	3243	OH2	TIP3			79.109	1.028	18.201		41.88
ATOM ATOM	3246	OH2	TIP3			59.332	-11.681	7.236		46.40
ATOM	3249	OH2	TIP3		2	13.967	-1.218	-4.268		63,45
ATOM	3252	OH2	TIP3			59.444	2.867	33.368		34.79
ATOM	3255	OH2	TIP3			32.024	13.487	19.852		41.00
ATOM	3258	OH2	TIP3	19	5	72.101	16.218	22.802		53.61
	3261	OH2	TIP3	19	6	0.987	-8.546	14.474		14.03
ATOM	3264	OH2	TIP3	19	7	-0.491	5.461	30.372		11.38
ATOM	3267	OH2	TIP3	198	3	61.179	6.795	11.905		88.51
ATOM	3270	OH2	TIP3	199		-1.365	-4.128	27.656		11.77
ATOM	3273	OH2	TIP3			81.440	15.558	17.262		0.98
ATOM	3276	OH2	TIP3	201	Ļ	-17.491	4.116	23.873		4.47
ATOM ATOM	3279	OH2	TIP3	202	?	27.546	10.513	14.499		0.58
ATOM ATOM	3282	OH2	TIP3	203		34.992	4.513	27.719		9.06
	3285	OH2	TIP3	204		-3.486	-4.591	9.171		9.89
MOTA	3288	OH2	TIP3	205		42.799	7.848	22.320		9.53
								-2.340	1.00 4	3.50

ATOM	3291	OH2	TIP3	206	52.728	11.884	21.811	1.00	39.98
MOTA	3294	OH2	TIP3	207	26.706	14.069	19.833	1.00	46.68
ATOM	3297	OH2	TIP3	208	-7.154	8.907	6.444	1.00	42.83
MOTA	3300	OH2	TIP3	209	86.648	5.606	16.034	1.00	51.15
ATOM	3303	OH2	TIP3	210	54.879	15.840	20.379	1.00	50.23
MOTA	3306	OH2	TIP3	211	51.417	19.473	22.691	1.00	48.35
ATOM	3309	OH2	TIP3	212	20.102	6.924	7.085	1.00	38.15
MOTA	3312	OH2	TIP3	213	28.991	1.941	-3.570	1.00	47.39
ATOM	3315	OH2	TIP3	214	26.505	2.386	-4.633	1.00	46.48
ATOM	3318	OH2	TIP3	215	36.482	2.810	18.521	1.00	46.26
MOTA	3321	OH2	TIP3	216	16.941	-20.504	14.128	1.00	49.74
MOTA	3324	OH2	TIP3	217	28.572	-14.448	6.157	1.00	49.13
MOTA	3327	OH2	TIP3	218	31.380	1.471	-1.998	1.00	43.02
MOTA	3330	OH2	TIP3	219	10.065	-16.338	15.455	1.00	42.75
ATOM	3333	OH2	TIP3	220	7.350	-11.974	5.652	1.00	55.35
ATOM	3336	OH2	TIP3	221	-12.328	14.547	10.986	1.00	51.29
ATOM	3339	OH2	TIP3	222	11.186	9.609	-1.388	1.00	37.68
ATOM	3342	OH2	TIP3	223	11.389	12.276	-1.400	1.00	46.93
MOTA	3345	OH2	TIP3	224	34.202	13.069	-1.161	1.00	41.79
MOTA	3348	OH2	TIP3	225	31.303	17.822	7.853	1.00	48.21
ATOM	3351	OH2	TIP3	226	36.875	11.804	-2.106	1.00	59.03
ATOM	3354	OH2	TIP3	227	35.134	3.048	11.020	1.00	50.41
ATOM	3357	OH2	TIP3	228	63.950	13.409	26.627	1.00	43.40
ATOM	3360	OH2	TIP3	229	36.367	6.116	15.221	1.00	57.79
ATOM	3363	OH2	TIP3	230	90.606	4.355	6.342	1.00	47.53
MOTA	3366	OH2	TIP3	231	50.038	-11.673	10.767	1.00	56.90
MOTA	3369	OH2	TIP3	232	60.196	-10.144	16.590	1.00	51.61
MOTA	3372	OH2	TIP3	233	18.021	-21.179	7.008	1.00	49.93
MOTA	3375	OH2	TIP3	234	66.236	-1.218	30.583	1.00	39.55
MOTA	3378	OH2	TIP3	235	74.959	18.928	20.659	1.00	38.04
ATOM	3381	OH2	TIP3	236	<sub>.</sub> -2.816	10.082	3.187	1.00	49.31
ATOM	3384	OH2	TIP3	237	5.894	-3.410	25.289	1.00	35. <b>5</b> 5
MOTA	3387	OH2	TIP3	238	35.784	6.047	12.543	1.00	41.96
MOTA	3390	OH2	TIP3	239	-5.400	16.537	14.180	1.00	43.13
MOTA	3393	OH2	TIP3	240	46.589	-11.622	26.970	1.00	43.71
MOTA	3396	OH2	TIP3	241	6.199	6.592	13.797	1.00	46.51
MOTA	3399	OH2	TIP3	242	-3.777	-5.158	20.907	1.00	42.08
MOTA	3402	OH2	TIP3	243	1.969	-3.711	-0.282	1.00	37.38
MOTA	3405	OH2	TIP3	244	86.200	11.629	22.877	1.00	56.51
MOTA	3408	OH2	TIP3		10.557	7.565	5.514	1.00	47.58
MOTA	3411	OH2	TIP3		4.802	8.149	2.136	1.00	50.70
MOTA	3414	OH2	TIP3		64.590	-8.128	20.596	1.00	43.65
ATOM	3417	OH2	TIP3		11.346	-17.840	13.283	1.00	47.64
ATOM	3420	OH2	TIP3	249	42.116	-6.808	14.953	1.00	53.79
ATOM	3423	OH2	TIP3	250	2.745	-4.054	22.128	1.00	60.88
ATOM	3426	OH2	TIP3	251	71.999	1.177	-2.124	1.00	47.90
ATOM	3429	OH2	TIP3	252	50.328	-3.210	33.068	1.00	57.01
MOTA	3435	OH2	TIP3	253	57.838	9.337	11.631	1.00	52.55
MOTA	3438	OH2	TIP3	254	43.373	20.489	30.490	1.00	51.97
MOTA	3441	OH2	TIP3	255	67.045	16.529	15.793	1.00	49.02
ATOM	3444	OH2	TIP3	256	87.509	21.566	5.114	1.00	54.21
MOTA	3447	OH2	TIP3	257	21.060	10.052	-9.215	1.00	60.32
MOTA	3450	OH2	TIP3	258	11.827	2.450	27.951	1.00	54.26
MOTA	3453	OH2	TIP3	259	64.788	-0.418	3.563	1.00	50.94



ATOM ATOM ATOM ATOM ATOM	3456 3459 3462 3465 3468	OH2 OH2 OH2 OH2 OH2	TIP3 TIP3 TIP3 TIP3	261 262 263 264	25.605 -18.804 30.652 22.350	28.473 -8.106 10.886 11.349 -16.098		1.00 1.00 1.00 1.00	62.81 52.81 55.25 50.40 53.27
ATOM	3471	OH2	TIP3			-16.098 9.106	-2.742 18.465	1.00 1.00	53.27 57.23

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## TABLE 2

Atom		Atom	A.A	A.A	x	Y	Z	occ	В
No.		Туре	Type	No.					
ATOM	1	N	GLU	1464	-13.425	16.769	8.973	1.00	61.21
ATOM	3	CA	GLU	1464	-12.536	16.852	7.821	1.00	59.70
ATOM	4	СВ	GLU	1464	-11.383	17.829	8.085	1.00	60.05
ATOM	5	С	GLU	1464	-11.998	15.478	7.427	1.00	57.11
ATOM	6	0	GLU	1464	-12.134	15.076	6.274	1.00	59.75
MOTA	7	N	LEU	1465	-11.406	14.749	8.368	1.00	52.21
MOTA	9	CA	LEU	1465	-10.871	13.424	8.062	1.00	46.72
MOTA	10	CB	LEU	1465	-10.102	12.844	9.249	1.00	44.98
MOTA	11	CG	LEU	1465	-8.608	13.123	9.384	1.00	46.11
ATOM	12	CD1	LEU	1465	-8.338	14.592	9.663	1.00	51.13
ATOM	13	CD2	LEU	1465	-8.064	12.286	10.512	1.00	4.99
ATOM	14	C	LEU	1465	-12.000	12.475	7.700	1.00	44.16
ATOM	15	0	LEU	1465	-13.101	12.577	8.239	1.00	44.04
ATOM	16	N	PRO	1466	-11.760	11.580	6.732	1.00	42.53
ATOM	17	CD	PRO	1466	-10.535	11.534	5.913	1.00	41.30
MOTA	18	CA	PRO	1466	-12.740	10.591	6.269	1.00	41.16
ATOM	19	CB	PRO	1466	-12.134	10.111	4.959	1.00	41.48
MOTA	20	CG	PRO	1466	-10.658	10.213	5.220	1.00	41.30
ATOM	21	С	PRO	1466	-12.906	9.441	7.261	1.00	41.31
MOTA	22	0	PRO	1466	-11.929	8.936	7.816	1.00	41.05
ATOM	23	N	GLU	1467	-14.145	9.044	7.500	1.00	41.02
ATOM	25	CA	GLU	1467	-14.428	7.960	8.427	1.00	42.42
MOTA	26	CB	GLU	1467	-15.931	7.904	8.712	1.00	47.98
MOTA	27	CG	GLU	1467	-16.565	9.238	9.105	1.00	52.79
MOTA	28	CD	GLU	1467	-17.998	9.093	9.606	1.00	54.21
MOTA	29	OE1	GLU	1467	-18.474	7.949	9.741	1.00	58.90
MOTA	30	OE2	GLU	1467	-18.650	10.120	9.879	1.00	55.90
MOTA	31	С	GLU	1467	-13.972	6.628	7.837	1.00	40.93
ATOM	32	0	GLU	1467	-14.061	6.426	6.620	1.00	44.32
ATOM	33	N	ASP	1468	-13.473	5.731	8.689	1.00	35.10
MOTA	35	CA	ASP	1468	-13.024	4.404	8.256	1.00	31.82
MOTA	36	CB	ASP	1468	-11.507	4.358	7.992	1.00	30.65
MOTA	37	CG	ASP	1468	-11.025	3.002	7.440	1.00	29.93
ATOM	38	OD1	ASP	1468	-11.689	1.958	7.603	1.00	29.63
ATOM	39	OD2	ASP	1468	-9.945	2.974	6.835	1.00	33.63
ATOM	40	C	ASP	1468	-13.394	3.441	9.369	1.00	31.81
MOTA	41	0	ASP	1468	-12.618	3.209	10.302	1.00	31.91
MOTA	42	N	PRO	1469	-14.569	2.819	9.247	1.00	29.68
ATOM	43	CD	PRO	1469	-15.482	2.963	8.097	1.00	28.33
ATOM	44	CA	PRO	1469	-15.100	1.863	10.220	1.00	31.80
MOTA	45	СВ	PRO	1469	-16.352	1.331	9.510	1.00	32.51
MOTA	46	CG	PRO	1469	-16.783	2.496	8.656	1.00	27.41
ATOM	47	C	PRO	1469	-14.146	0.731	10.590	1.00	30.44
MOTA	48	0	PRO	1469	-14.272	0.135	11.654	1.00	30.02
MOTA	49	N	ARG	1470	-13.198	0.442	9.704	1.00	31.06
ATOM	51	CA	ARG	1470	-12.240	-0.636	9.917	1.00	31.86
ATOM	52	СВ	ARG	1470	-11.386	-0.860	8.660	1.00	31.36
ATOM	53	CG	ARG	1470	-12.107	-1.437	7.448	1.00	33.08

	TOM 5	_	D AR	3 1470	-11.14	0 . ~			
	rom 5	5 <b>N</b>		_		_	–	48 1.0	00 31.08
	rom 5	7 C		_		_		91 1.0	
ΑŢ	COM 5	3 N	H1 ARC	•	05		~	19 1.0	
ΑT	OM 6	L NI	H2 ARG		-9.26			35 1.0	0 35.90
ΓA	OM 64	L C	ARG		-9.15				
AT	'OM 65		ARG		-11.29			95 1.0	
AT	OM 66	N	TRP		-10.82		.0 11.68		
AT	OM 68			_	-11.03		4 11.45		
AT	OM 69				-10.063		0 12.50		
AT	OM 70				-8.816		7 11.85		
ATO		CD		1471	-8.173		5 10.94		
ATO		CE		1471	-7.288		9 11.31		_
ATO		CE		1471	-6.913	-0.99	2 10.13		,
ATO		CD:		1471	-6.762	-0.76			
ATC		NE:		1471	-8.309	0.666			
ATO	. •	CZ		1471	-7.557	-0.373			
ATO		CZ		1471	-6.042	-2.085			
АТО				1471	-5.897	-1.853			
ATO		CH2		1471	-5.541	-2.494			-2.03
ATO		C	TRP	1471	-10.477	2.019			30.18
ATO		0	TRP	1471	-9.782	2.108		-	29.94
ATO		N	GLU	1472	-11.573	2.737		_	30.00
ATON		CA	GLU	1472	-12.051	3.706			29.06
ATON		CB	GLU	1472	-13.312	4.386	13.849		28.62
ATOM		CG	GLU	1472	-13.641	5.733	14.529		29.16
ATOM	• .	CD	GLU	1472	-12.676	6.848	14.156	1.00	30.74
ATOM		OE1	GLU	1472	-12.090	6.799	13.057	1.00	30.05
ATOM		OE2	GLU	1472	-12.511	7.784	14.961	1.00	31.32
ATOM		C	GLU		-12.327	3.159	15.767	1.00	30.26
ATOM		0	GLU		-12.969	2.125	15.916	1.00	28.70
ATOM		N	LEU	1473	-11.810	3.842	16.781	1.00	31.01
ATOM		CA		<b>147</b> 3 .	-12.054	3.451	18.161	1.00	27.38
ATOM		CB			-10.763	3.073	18.899	1.00 1.00	29.61
ATOM	97	CG			-10.923	2.756	20.403	1.00	28.56
ATOM	98	CD1			11.485	1.354	20.639	1.00	30.06
ATOM	99	CD2 C	-	1473	-9.595	2.876	21.115	1.00	28.42
ATOM	100				12.617	4.714	18.764	1.00	28.15
ATOM	101	O N			12.179	5.814	18.407	1.00	31.81
ATOM	102			1474 -	13.670	4.591	19.596	1.00	33.00
ATOM	102	CD			14.488	3.400	19.859		31.45
ATOM	103	CA			14.261	5.774	20.226		31.72
ATOM	105	CB			15.400	5.176	21.048		31.23
ATOM	106	CG			15.815	4.005	20.247		29.01
ATOM	100	C		.474 -	13.217	6.444	21.120	_	29.09
ATOM	108	0		474 -	12.447	5.765	21.808		33.36
ATOM		N		475 -	13.188	7.770	21.112		36.40
ATOM	110	CA			12.228	8.498			33.67
ATOM	111	CB			L2.433		21.735		33.96
ATOM	112				2.134				35.31
ATOM	113			475 -1	2.060				10.10
ATOM	114				1.785				2.98
ATOM	116				0.578	4.0			12.91
ATOM	117					10			1.30
221 OM	120	NH2	ARG 14						1.88
CCCD /= -					-	.=.507	16.943	1.00 4	0.98

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ATOM	123	C	ARG	1475	-12.278	8.142	23.404	1.00	35.88
ATOM	124	0	ARG	1475	-11.240	8.046	24.061	1.00	37.10
ATOM	125	N	ASP	1476	-13.479	7.920	23.928	1.00	36.47
ATOM	127	CA	ASP	1476	-13.632	7.581	25.335	1.00	37.24
ATOM	128	CB	ASP	1476	-15.112	7.629	25.741	1.00	39.66
ATOM	129	CG	ASP	1476	-15.930	6.480	25.163	1.00	42.38
MOTA	130	OD1	ASP	1476	-15.438	5.706	24.322	1.00	47.52
ATOM	131	OD2	ASP	1476	-17.098	6.349	25.568	1.00	48.06
ATOM	132	С	ASP	1476	-13.023	6.232	25.724	1.00	36.93
MOTA	133	0	ASP	1476	-13.034	5.856	26.898	1.00	40.09
MOTA	134	N	ARG	1477	-12.564	5.475	24.732	1.00	34.34
ATOM	136	CA	ARG	1477	-11.961	4.171	24.993	1.00	32.47
MOTA	137	CB	ARG	1477	-12.269	3.212	23.852	1.00	31.59
MOTA	138	CG	ARG	1477	-13.716	2.939	23.640	1.00	29.66
ATOM	139	CD	ARG	1477	-14.314	2.342	24.875	1.00	30.65
MOTA	140	NE	ARG	1477	-14.498	3.342	25.918	1.00	31.37
ATOM	142	CZ	ARG	1477	-14.822	3.055	27.174	1.00	32.81
MOTA	143	NHl	ARG	1477	-15.002	1.794	27.549	1.00	33.92
ATOM	146	NH2	ARG	1477	-14.950	4.025	28.062	1.00	31.74
ATOM	149	С	ARG	1477	-10.452	4.266	25.153	1.00	33.13
MOTA	150	0	ARG	1477	-9.777	3.281	25.445	1.00	33.55
MOTA	151	N	LEU	1478	-9.923	5.466	24.984	1.00	34.43
ATOM	153	CA	LEU	1478	-8.493	5.663	25.076	1.00	35.68
MOTA	154	CB	LEU	1478	-8.008	6.350	23.790	1.00	34.98
ATOM	155	CG	LEU	1478	-6.581	6.137	23.284	1.00	31.11
ATOM	156	CD1	LEU	1478	-6.280	4.650	23.161	1.00	26.62
ATOM	157	CD2	LEU	1478	-6.428	6.839	21.940	1.00	28.80
MOTA	158	С	LEU	1478	-8.158	6.505	26.295	1.00	36.21
MOTA	159	0	LEU	1478	-8.501	7.688	26.361	1.00	39.67
MOTA	160	N	VAL	1479	-7.558	5.878	27.293	1.00	35.42
MOTA	162	CA	VAL	1479	-7.156	6.599	28.491	1.00	35.80
MOTA	163	CB	VAL	1479	-7.269	5.707	29.742	1.00	36.29
ATOM	164	CG1	VAL	1479	-7.017	6.527	30.983	1.00	37.23
MOTA	165	CG2	VAL	1479	-8.650	5.059	29.812	1.00	34.41
ATOM	166	С	VAL	1479	-5.704	7.046	28.244	1.00	35.68
MOTA	167	0	VAL	1479	-4.764	6.246	28.319	1.00	33.45
MOTA	168	N	LEU	1480	-5.538	8.315	27.885	1.00	38.15
ATOM	170	CA	LEU	1480	-4.213	8.860	27.584	1.00	42.61
MOTA	171	CB	LEU	1480	-4.332	10.205	26.857	1.00	39.14
MOTA	172	CG	LEU	1480	-4.969	10.179	25.460	1.00	38.44
MOTA	173	CD1	LEU	1480	-4.901	11.579	24.879	1.00	39.39
MOTA	174	CD2	LEU	1480	-4.263	9.194	24.533	1.00	36.86
MOTA	175	С	LEU	1480	-3.274	8.970	<b>28.7</b> 83	1.00	46.37
MOTA	176	0	LEU	1480	-3.659	9.445	29.850	1.00	48.86
ATOM	177	N	GLY	1481	-2.033	8.537	28.594	1.00	47.13
MOTA	179	CA	GLY	1481	-1.081	8.573	29.678	1.00	48.19
ATOM	180	С	GLY	1481	0.163	9.388	29.425	1.00	50.27
MOTA	181	0	GLY	1481	0.152	10.367	28.675	1.00	51.19
ATOM	182	N	LYS	1482	1.240	8.965	30.078	1.00	50.93
MOTA	184	CA	LYS	1482	2.543	9.606	30.007	1.00	50.94
MOTA	185	CB	LYS	1482	3.509	8.866	30.933	1.00	50.41
MOTA	186	CG	LYS	1482	4.971	9.026	30.567	1.00	51.87
ATOM	187	CD	LYS	1482	5.810	7.874	31.087	1.00	53.49
ATOM	188	CE	LYS	1482	5.390	6.542	30.478	1.00	50.77

ΓA	COM 1	89	N#77 .								
			_	LYS	1482			133 30.	986	1 00	
			_	LYS	1482	3.14	5 9.6			1.00	
			_	YS	1482	3.119	5 8.7			1.00	51
AT	_			PRO	1483	3.706	10.8			1.00	52.30
AT		`			1483	3.667	12.1			1.00	53.47
AT		`			1483	4.326	11.0			1.00	54.19
ATO					1483	4.772	12.4			1.00	54.10
ATO					1483	3.772				1.00	54.25
ATO			-		L483	5.535	10.0			00	55.30
ATO	•		_		1483	6.343	10.0			.00	54.72
ATC					484	5.619	9.3			.00	53.48
ATO					484	6.739	8.44			.00	57.05
ATO			_		484	6.307	7.24			.00	59.26
ATO					484	5.391	6.21			.00	59.35
ATO				_	484	4.975	5.16			.00	60.87
ATO				_	484	6.081	5.57			.00	57.14
ATO		. •	LE	_	484	7.847	9.19			.00	59.79
ATO		•	LE	_	484	8.980	8.72			.00	61.30
ATO			GL		485	7.494	10.35		_	00	62.17
ATOM			GL	Y 1	185	8.456	11.17			00	63,75
ATOM	_	_	GL	Y 14	185	8.081	11.41			00	66.33
ATOM		_	GL.		85	6.918	11.65	_		00	67.79
ATOM			GLi		91	4.615	13.76				69.61
ATOM		CA	GLI		91	4.353	13.353				58.26
ATOM		CB	GLI		91	3.476	14.379		_		57.98
ATOM		CG	GLM		91	3.134	14.034				61.80
ATOM		CD	GLN			2.019	14.911	22			70.31
ATOM		OE 1				1.355	15.636				75.91
ATOM	223 226	NE2			91	1.820	14.832		_		77.85
ATOM	227	C	GLN			3.709	11.965	19.88			78.30
ATOM	228	0	GLN	14	91	2.701	11.669	19.222		_	54.67
ATOM	230	N	VAL	149		4.305	11.125	20.729		_	54.91
ATOM	231	CA	VAL	149		3.825	9.763	20.723	_		0.04
ATOM	232	CB	VAL	149		4.861	8.705	20.583			4.93
ATOM	232	CG1	VAL	149	2	4.378	7.325	20.958			2.65
ATOM	234	CG2	VAL	149		5.119	8.766	19.099			9.71
ATOM	235	C	VAL	149		3.584	9.661	22.490	_	_	0.98
ATOM	236	0	VAL	149		4.451	10.029	23.289	1.0		3.43
ATOM	238	N	VAL	149		2.400	9.212	22.888	1.00		3.43
ATOM	239	CA CB	VAL	149		2.107	9.080	24.304	1.00		1.13
ATOM	240		VAL	149		1.052	10.133	24.782	1.00		8.77
ATOM	241	CG1 CG2	VAL	149		1.410	11.508	24.287	1.00		6.35
ATOM	242	CG2	VAL	149		-0.329	9.755	24.339			5.06
ATOM	243		VAL	149		1.589	7.693	24.619	1.00		7.64
ATOM	244	0	VAL	149		0.948	7.058	23.783	1.00		7.77
ATOM	246	N	LEU	1494		1.949	7.187	25.790	1.00		3.88
ATOM	247	CA	LEU	1494		1.468	5.880	26.205	1.00		. 24
ATOM		CB	LEU	1494		2.252	5.383	27.429	1.00	_	.92
ATOM	248	CG	LEU	1494	:	1.886	4.009	28.004	1.00		.41
	249	CD1	LEU	1494		1.927	2.931	26.924	1.00	•	.21
<b>-</b> · ·	250	CD2	LEU	1494		2.835	3.670	29.145	1.00		.60
	251	C	LEU	1494	-	0.010	6.095	26.564	1.00		.03
	252	0	LEU	1494	-	0.425	7.215	26.887	1.00		. 27
····	253	N	ALA	1495		0.807	5.043		1.00		. 35
SSSD/551	145 6:							26.468	1.00	34.	. 93



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ATOM	255	CA	ALA	1495	-2.220	5.145	26.768	1.00	34.44
ATOM	256	CB	ALA	1495	-2.955	5.794	25.616	1.00	35.29
ATOM	25.7	С	ALA	1495	-2.781	3.770	27.018	1.00	34.59
MOTA	258	0	ALA	1495	-2.128	2.766	26.748	1.00	35.52
MOTA	259	N	GLU	1496	-3.996	3.723	27.536	1.00	36.64
ATOM	261	CA	GLU	1496	-4.652	2.462	27.806	1.00	37.57
MOTA	262	CB	GLU	1496	-5.000	2.354	29.287	1.00	38.97
MOTA	263	CG	GLU	1496	-3.769	2.304	30.185	1.00	41.79
MOTA	264	CD	GLU	1496	-4.110	2.475	31.645	1.00	43.65
MOTA	265	OE1	GLU	1496	-4.408	3.617	32.036	1.00	42.97
MOTA	266	OE2	GLU	1496	-4.086	1.475	32.398	1.00	46.65
MOTA	267	C	GLU	1496	-5.896	2.404	26.943	1.00	38.50
MOTA	268	0	GLU	1496	-6.660	3.371	26.867	1.00	40.28
MOTA	269	N	ALA	1497	-6.051	1.301	26.223	1.00	37.34
MOTA	271	CA	ALA	1497	-7.194	1.131	25.352	1.00	37.42
MOTA	272	CB	ALA	1497	-6.743	0.625	23.985	1.00	35.92
MOTA	273	C	ALA	1497	-8.146	0.148	26.000	1.00	36.77
MOTA	274	0	ALA	1497	-7.759	-0.977	26.323	1.00	35.74
MOTA	275	N	ILE	1498	-9.354	0.616	26.291	1.00	37.03
MOTA	277	CA	ILE	1498	-10.378	-0.224	26.896	1.00	36.80
MOTA	278	CB	ILE	1498	-11.372	0.612	27.728	1.00	34.53
ATOM	279	CG2	ILE	1498	-12.373	-0.290	28.425	1.00	34.59
ATOM	280	CG1	ILE	1498	-10.640	1.438	28.778	1.00	31.97
ATOM	281	CD1	ILE	1498	-11.552	2.344	29.541	1.00	31.12
ATOM	282	С	ILE	1498	-11.126	-0.807	25.709	1.00	38.72
MOTA	283	0	ILE	1498	-11.647	-0.066	24.879	1.00	37.74
MOTA	284	N	GLY	1499	-11.137	-2.126	25.590	1.00	40.98
ATOM	286	CA	GLY	1499	-11.839	-2.728	24.482	1.00	44.64
ATOM	287	С	GLY	1499	-10.931	-3.115	23.332	1.00	48.45
MOTA	288	0	GLY	1499	-10.260	-4.147	23.401	1.00	51.92
MOTA	289	N	LEU	1500	-10.877	-2.269	22.303	1.00	47.87
MOTA	291	CA	LEU	1500	-10.076	-2.530	21.102	1.00	46.80
MOTA	292	CB	LEU	1500	-8.594	-2.770	21.434	1.00	45.37
MOTA	293	CG	LEU	1500	-7.543	-1.661	21.293	1.00	44.84
ATOM	294	CD1	LEU	1500	-6.174	-2.290	21.450	1.00	43.33
ATOM	295	CD2	LEU	1500	-7.623	-0.959	19.948	1.00	40.43
ATOM	296	С	LEU	1500	-10.631	-3.737	20.349	1.00	45.63
ATOM	297	0	LEU	1500	-10.797	-4.823	20.915	1.00	44.42
ATOM	298	N	PRO	1505	-13.569	-5.910	25.549	1.00	52.13
ATOM	299	CD	PRO	1505	-14.316	-7.170	25.398	1.00	54.09
ATOM	300	CA	PRO	1505	-14.451	-4.828	25.999	1.00	50.46
MOTA	301	CB	PRO	1505	-15.841	-5.455	25.891	1.00	49.86
ATOM	302	CG	PRO	1505	-15.586	-6.898	26.193	1.00	52.17
MOTA	303	C	PRO	1505	-14.136	-4.370	27.422	1.00	47.75
MOTA	304	0	PRO	1505	-14.148	-3.180	27.710	1.00	47.93
ATOM	305	N	ASN	1506	-13.778	-5.313	28.285	1.00	46.20
MOTA	307	CA	ASN	1506	-13.458	-4.986	29.666	1.00	49.52
MOTA	308	CB	ASN	1506	-14.310	-5.829	30.612	1.00	52.42
ATOM	309	CG	ASN	1506	-15.788	-5.489	30.526	1.00	54.50
MOTA	310	OD1	ASN	1506	-16.179	-4.331	30.680	1.00	57.16
MOTA	311	ND2	ASN	1506	-16.610	-6.489	30.244	1.00	56.82
MOTA	314	С	ASN	1506	-11.973	-5.124	30.003	1.00	50.65
MOTA	315	0	ASN	1506	-11.583	-5.174	31.178	1.00	50.65
ATOM	316	N	ARG	1507	-11.142	-5.145	28.968	1.00	50.90



			CA	ARG	1507	-9.700	٠			
			CB	ARG	1507					00 49.77
				ARG	1507					00 55.81
		21 (	CD .	ARG	1507	-8.408	_			00 61.63
		22		ARG	1507	-8.600	–			00 66.01
	OM 32			ARG	1507	-8.004				00 72.55
AT		25 N		ARG	1507	-7.198	-9.9			00 77.32
AT		8 N		<b>I</b> RG	1507	-8.335	-9.16			00 78.41
ATO		1 0		<b>I</b> RG	1507	-9.015	-11.19			00 79.30
ATO		2 0		LRG	1507	-9.452	-4.03			00 45.60
ATO		3 N	ν	'AL	1508	-7.977	-3.46			00 42.08
ATO		5 C.	A v	AL	1508	-7.216	-3.59			
ATC		6 C		ΆL	1508	-6.903	-2.44			0 40.75
ATC			31 V	AL	1508	-8.303	-1.42			00 38.75
ATO		3 C(	32 V.	AL	1508	-5.919	-1.01			0 43.29
ATO		<b>∂</b> C	V.	AL	1508	-5.929	-2.00		.2 1.0	0 37.56
ATO		0	V	AL	1508	-5.369	-2.97		•	0 39.14
ATO		N		IR.	1509	-5.517	-3.97	-		0 39.16
ATO		CA	T	IR .	1509	-4.298	-2.349			
ATO	_	CE	TH		1509	-4.571	-2.731			0 36.52
ATO			1 TH		1509	-5.423	-3.187			0 37.83
ATON			2 TH		1509	-3.267	-4.340			
ATON		C	TH		1509	-3.434	-3.540			34.51
ATOM		0	TH		1509	-3.927	-1.495			
ATOM		N	LY		1510	-2.175	-0.408			
ATOM		CA	LY	_	1510	-1.291	-1.628			35.96
ATOM		CB	LY.	S ]	1510	-0.032	-0.479		_	
ATOM		CG	LY:	S 1	510	-0.277	-0.695 -0.854	27.680		
ATOM		CD	LY	5 1	510	1.023	-0.658	29.162		
ATOM ATOM		CE	LYS	3 1	510	0.947	-1.286	29.948		55
ATOM		NZ	LYS	3 1	510	-0.149	-0.728	31.342	-	
ATOM		C	LYS		510	-0.929	-0.355	32.187 25.373		64.94
ATOM	362	0	LYS		510	-0.574	-1.345	24.734	1.00	34.59
ATOM	363 365	N	VAL		511	~1.092	0.846	24.835	1.00	31.43
ATOM	366	CA	VAL		511	-0.810	1.121	23.441	1.00	32.95
ATOM	367	CB	VAL		511	-2.129	1.213	22.621	1.00	32.29
ATOM	368	CG1	VAL		511	-2.879	-0.109	22.686	1.00	32.95
ATOM	369	CG2	VAL		511	-3.026	2.354	23.148	1.00 1.00	34.79
ATOM	370	C	VAL		511	-0.058	2.446	23.353	1.00	32.84
ATOM	371	0	VAL		511	0.021	3.185	24.344	1.00	32.65
ATOM	373	N	ALA		12	0.521	2.721	22.186	1.00	31.62
ATOM	374	CA CB	ALA		12	1.244	3.969	21.954	1.00	30.24
ATOM	375	CB	ALA		12	2.599	3.700	21.316	1.00	28.18
ATOM	376	0	ALA		12	0.373	4.783	21.015	1.00	25.62
ATOM	377	Ŋ	ALA			-0.151	4.264	20.040	1.00	27.54
MOTA	379		VAL	15		0.204	6.054	21.322	1.00	27.17
ATOM	380	CA	VAL	15		-0.630	6.914	20.503	1.00	30.52
ATOM	381	CB	VAL	15		-1.731	7.591	21.347	1.00	34.08
ATOM	382	CG1	VAL	15.		2.607	8.444	20.474	1.00	34.61
ATOM	383	CG2	VAL	15		2.567	6.549	22.087	1.00	36.75
ATOM	384	C O	VAL	15:		0.203	8.008	19.837	1.00	33.45
ATOM	385	N	VAL	15:		0.924	8.750	20.510	1.00	36.38
ATOM	387		LYS	151		0.105		18.513	1.00	35.32
•	507	CA	LYS	151	.4	0.818		17.746	1.00	38.19
									4.00	40.12

ATOM	388	CB	LYS	1514	1.339	8.513	16.439	1.00	40.93
ATOM	389	CG	LYS	1514	2.452	7.488	16.632	1.00	42.52
ATOM	390	CD	LYS	1514	2.861	6.803	15.338	1.00	46.25
ATOM	391	CE	LYS	1514	3.268	7.796	14.261	1.00	49.76
ATOM	392	NZ	LYS	1514	4.304	8.771	14.705	1.00	52.14
ATOM	396	С	LYS	1514	-0.166	10.215	17.458	1.00	40.69
MOTA	397	0	LYS	1514	-1.313	9.953	17.110	1.00	41.69
ATOM	398	N	MET	1515	0.277	11.454	17.613	1.00	43.28
ATOM	400	CA	MET	1515	-0.569	12.610	17.379	1.00	46.21
ATOM	401	CB	MET	1515	-1.363	12.936	18.644	1.00	46.96
ATOM	402	CG	MET	1515	-0.488	13.293	19.837	1.00	47.61
ATOM	403	SD	MET	1515	-1.413	13.464	21.358	1.00	49.77
ATOM	404	CE	MET	1515	-1.593	11.761	21.814	1.00	47.84
MOTA	405	С	MET	1515	0.299	13.805	17.000	1.00	49.90
MOTA	406	0	MET	1515	1.519	13.788	17.194	1.00	49.83
ATOM	407	N	LEU	1516	-0.339	14.822	16.430	1.00	54.45
ATOM	409	CA	LEU	1516	0.335	16.053	16.023	1.00	57.57
MOTA	410	CB	LEU	1516	-0.483	16.762	14.944	1.00	54.10
MOTA	411	CG	LEU	1516	-0.800	16.007	13.664	1.00	50.71
ATOM	412	CD1	LEU	1516	-1.830	16.800	12.901	1.00	51.20
ATOM	413	CD2	LEU	1516	0.467	15.809	12.849	1.00	50.08
ATOM	414	С	LEU	1516	0.487	17.010	17.202	1.00	61.88
MOTA	415	0	LEU	1516	-0.170	16.852	18.235	1.00	63.30
MOTA	416	N	LYS	1517	1.335	18.018	17.021	1.00	66.83
ATOM	418	CA	LYS	1517	1.568	19.036	18.037	1.00	71.46
MOTA	419	CB	LYS	1517	2.985	19.593	17.911	1.00	76.28
ATOM	420	CG	LYS	1517	4.084	18.626	18.349	1.00	82.19
MOTA	421	CD	LYS	1517	5.450	19.085	17.846	1.00	86.93
ATOM	422	CE	LYS	1517	6.579	18.228	18.411	1.00	90.46
MOTA	423	NZ	LYS	1517	7.896	18.513	17.763	1.00	92.51
MOTA	427	C	LYS	1517	0.549	20.156	17.837	1.00	72.44
MOTA	428	0	LYS	1517	-0.142	20.198	16.819	1.00	72.12
MOTA	429	N	SER	1518	0.474	21.075	18.793	1.00	73.90
ATOM	431	CA	SER	1518	-0.470	22.185	18.697	1.00	74.96
MOTA	432	CB	SER	1518	-0.498	22.980	20.002	1.00	74.72
MOTA	433	C	SER	1518	-0.133	23.100	17.525	1.00	76.16
ATOM	434	0	SER	1518	-1.029	23.667	16.897	1.00	76.56
ATOM	435	N	ASP	1519	1.158	23.245	17.232	1.00	77.24
ATOM	437	CA	ASP	1519	1.601	24.094	16.125	1.00	78.51
ATOM	438	CB	ASP	1519	2.849	24.888	16.535	1.00	79.70
MOTA	439	C	ASP	1519	1.887	23.264	14.865	1.00	78.29
MOTA	440	0	ASP	1519	2.797	23.580	14.088	1.00	78.52
ATOM	441	N	ALA	1520	1.121	22.192	14.682	1.00	76.90
ATOM	443	CA	ALA	1520	1.285	21.313	13.529	1.00	74.09
MOTA	444	CB	ALA	1520	0.737	19.930	13.840	1.00	74.20
MOTA	445	С	ALA	1520	0.580	21.895	12.318	1.00	71.82
ATOM	446	0	ALA	1520	-0.573	22.311	12.400	1.00	71.78
MOTA	447	N	THR	1521	1.291	21.951	11.202	1.00	69.97
MOTA	449	CA	THR	1521	0.734	22.480	9.970	1.00	68.86
MOTA	450	CB	THR	1521	1.848	22.911	9.026	1.00	68.87
MOTA	451	OG1	THR	1521	2.621	21.762	8.651	1.00	70.03
MOTA	453	CG2	THR	1521	2.756	23.912	9.715	1.00	71.55
MOTA	454	С	THR	1521	-0.081	21.389	9.292	1.00	67.89
ATOM	455	0	THR	1521	0.111	20.204	9.563	1.00	69.03



ATO			GL	J 1522	-0.964	21.78	3 8.38	2 1.00	
ATO				J 1522	-1.785				
ATO			GLU	J 1522	-2.737				_
ATO			GLU	J 1522	-0.886				
ATO		0	GLU	1522	-1.324				
ATO		N	LYS	1523	0.367				
ATO		CA	LYS	1523	1.314	19.326			
ATO	465	CB	LYS	1523	2.629	20.064			
ATON	466	CG	LYS	1523	3.815	19.162			
NOTA	467	CD	LYS		3.510	18.288			
ATOM	468	CE	LYS	_	4.759				
MOTA	1 469	NZ	LYS		4.429	17.596			65.88
ATOM	1 473	С	LYS	_	1.565	16.721	_		70.37
ATOM	474	0	LYS	1523	1.548	18.173			54.80
ATOM	475	N	ASP	1524	1.786	17.003			54.44
ATOM	477	CA	ASP	1524	2.036	18.523		1.00	51.67
ATOM	478	СВ	ASP	1524	2.036	17.549		1.00	49.43
MOTA	479	CG	ASP	1524		18.271		1.00	51.06
MOTA	480	OD1		1524	3.598	19.080	10.613	1.00	54.03
ATOM	481	OD2	ASP	1524	3.649	20.136	11.283	1.00	56.32
ATOM	482	C	ASP	1524	4.580	18.658	9.956	1.00	56.02
ATOM	483	ō	ASP	1524	0.847	16.596	9.413	1.00	47.73
ATOM	484	N	LEU	1525	1.017	15.387	9.580	1.00	45.85
ATOM	486	CA	LEU		-0.354	17.155	9.300	1.00	47.62
ATOM	487	СВ	LEU	1525 1525	-1.585	16.380	9.354	1.00	45.95
ATOM	488	CG	LEU		-2.801	17.307	9.271	1.00	43.61
ATOM	489	CD1	LEU	1525	-4.193	16.665	9.234	1.00	44.56
ATOM	490	CD2	LEU	1525	-4.364	15.543	10.268	1.00	46.02
ATOM	491	C	LEU	1525	-5.215	17.740	9.468	1.00	43.80
ATOM	492	o	LEU	1525	~1.605	15.372	8.210	1.00	45.67
ATOM	493	N	SER	1525	-1.921	14.204	8.416	1.00	46.78
ATOM	495	CA		1526	-1.245	15.822	7.014	1.00	45.44
ATOM	496	CB	SER	1526	-1.211	14.945	5.851	1.00	46.33
ATOM	497	OG	SER	1526	-0.903	15.744	4.584	1.00	48.48
ATOM	499	C	SER	1526	-2.012	16.546	4.218	1.00	57.28
ATOM	500	0	SER	1526	-0.192	13.821	5.995	1.00	43.84
ATOM	501	N	SER	1526	-0.480	12.669	5.674	1.00	45.24
ATOM	503	CA	ASP	1527	0.994	14.144	6.489	1.00	40.88
ATOM	504	CB	ASP	1527	2.024	13.128	6.646	1.00	39.70
ATOM	505		ASP	1527	3.376	13.767	6.960	1.00	37.62
ATOM	506	CG OD1	ASP	1527	3.934	14.555	5.786	1.00	37.01
ATOM	507	OD2	ASP	1527	3.399	14.434	4.657	1.00	35.78
ATOM	508	C C	ASP	1527	4.916	15.295	5.992	1.00	40.23
ATOM	509		ASP	1527	1.652	12.053	7.659	1.00	38.51
ATOM	510	0	ASP	1527	1.951	10.872	7.461	1.00	37.68
ATOM	512	N	LEU	1528	0.973	12.460	8.725	1.00	38.16
ATOM		CA	LEU	1528	0.532	11.513	9.744		38.29
	513	CB	LEU	1528	0.026	12.258	10.985		37.12
ATOM	514	CG	LEU	1528	-0.505	11.412			39.03
ATOM	515	CD1	LEU	1528	0.499	10.323			
ATOM	516	CD2	LEU	1528	-0.825	12.315			35.39
ATOM	517	С		1528	-0.568	10.611			35.29
ATOM	518	0	LEU	1528	-0.607	9.400	_		38.10
ATOM	519	N	ILE	1529	-1.450	11.210	_		37.21
ATOM	521	CA	ILE	1529	-2.531	10.472			36.71
					· <del>-</del>		, , , 18	1.00	35.93

MOTA	522	CB	ILE	1529	-3.486	11.419	6.931	1.00	35.67
MOTA	523	CG2	ILE	1529	-4.492	10.619	6.119	1.00	34.04
ATOM	524	CG1	ILE	1529	-4.259	12.295	7.916	1.00	33.81
ATOM	525	CD1	ILE	1529	-5.177	13.288	7.276	1.00	33.58
MOTA	526	С	ILE	1529	-1.912	9.447	6.786	1.00	37.49
ATOM	527	0	ILE	1529	-2.274	8.269	6.829	1.00	37.11
MOTA	528	N	SER	1530	-0.926	9.893	6.003	1.00	38.20
MOTA	530	CA	SER	1530	-0.217	9.036	5.050	1.00	37.49
ATOM	531	CB	SER	1530	0.911	9.822	4.370	1.00	43.32
ATOM	532	OG	SER	1530	0.424	10.970	3.687	1.00	52.31
MOTA	534	С	SER	1530	0.382	7.808	5.719	1.00	34.40
ATOM	535	0	SER	1530	0.234	6.691	5.219	1.00	31.51
ATOM	536	N	GLU	1531	1.048	8.028	6.851	1.00	32.08
ATOM	538	CA	GLU	1531	1.690	6.952	7.594	1.00	30.60
ATOM	539	CB	GLU	1531	2.506	7.515	8.759	1.00	29.70
ATOM	540	CG	GLU	1531	3.094	6.428	9.657	1.00	30.53
ATOM	541	CD	GLU	1531	3.871	6.962	10.839	1.00	33.17
MOTA	542	OE1	GLU	1531	4.473	6.134	11.552	1.00	33.38
ATOM	543	OE2	GLU	1531	3.883	8.193	11.062	1.00	37.52
ATOM	544	С	GLU	1531	0.698	5.911	8.094	1.00	30.17
ATOM	545	0	GLU	1531	0.991	4.714	8.100	1.00	29.76
ATOM	546	N	MET	1532	-0.464	6.379	8.530	1.00	31.34
MOTA	548	CA	MET	1532	-1.521	5.496	9.015	1.00	30.72
ATOM	549	CB	MET	1532	-2.666	6.336	9.591	1.00	29.99
ATOM	550	CG	MET	1532	-3.880	5.523	10.020	1.00	30.10
ATOM	551	SD	MET	1532	-5.173	6.510	10.727	1.00	29.46
ATOM	552	CE	MET	1532	-5.462	7.682	9.455	1.00	23.76
ATOM	553	C	MET	1532	-2.025	4.638	7.843	1.00	30.47
ATOM	554	0	MET	1532	-2.080	3.401	7.925	1.00	27.05
ATOM	555	N	GLU	1533	-2.387	5.319	6.756	1.00	30.56
ATOM	557	CA	GLU	1533	-2.863	4.674	5.542	1.00	30.56
ATOM	558	CB	GLU	1533	-3.090	5.725	4.458	1.00	28.60
ATOM	559	CG	GLU	1533	-4.226	6.677	4.761	1.00	29.08
ATOM	560	CD	GLU	1533	-5.531	5.954	5.014	1.00	31.28
ATOM	561	OE1	GLU	1533	-6.006	5.230	4.117	1.00	33.09
ATOM	562	OE2	GLU	1533	-6.086	6.104	6.121	1.00	34.97
ATOM	563	С	GLU	1533	-1.861	3.638	5.064	1.00	29.86
ATOM	564	0	GLU	1533	-2.232	2.541	4.677	1.00	32.28
ATOM	565	N	MET	1534	-0.590	4.014	5.107	1.00	32.54
MOTA	567	CA	MET	1534	0.515	3.145	4.719	1.00	33.39
ATOM	568	CB	MET	1534	1.826	3.894	4.885	1.00	34.70
ATOM	569	CG	MET	1534	3.038	3.047	4.654	1.00	44.51
ATOM	570	SD	MET	1534	3.479	3.063	2.943	1.00	52.81
MOTA	571	CE	MET	1534	4.349	4.607	2.874	1.00	47.34
ATOM	572	C	MET	1534	0.530	1.896	5.607	1.00	
ATOM	573	Ō	MET	1534	0.689	0.776	5.115	1.00	32.98
MOTA	574	N	MET	1535	0.364	2.100			34.00
MOTA	576	CA	MET	1535	0.336	0.986	6.910 7.848	1.00	31.92
ATOM	577	CB	MET	1535	0.330			1.00	30.80
ATOM	578	CG	MET	1535	1.509	1.503 2.216	9.294	1.00	33.77
ATOM	579	SD	MET	1535	1.520		9.810	1.00	32.26
ATOM	580	CE	MET	1535	1.183	2.433	11.617	1.00	34.75
ATOM	581	C	MET	1535	-0.837	4.173	11.723	1.00	37.86
ATOM	582	0	MET	1535		0.052	7.521	1.00	30.80
	-02	J	Little		-0.704	-1.175	7.589	1.00	32.03



ATO		N	LY	S 1536	-1.97	4 0.63	0 734		
ATO			LY	S 1536	-3.17				
ATO	•	CB	LY		-4.33		• • • •		
ATO:	M 587	CG	LY		-4.86				
ATO	M 588	CD	LY		-5.97		_		
ATO	M 589	CE			-6.43				
ATO	M 590	NZ	LY		-7.57				
OTA	1 594	C	LYS		-2.88				
OTA	1 595	0	LYS						30.71
ATON	1 596	N	MET		-3.238 -2.309	- · - · -			34.73
ATOM	1 598	CA	MET						31.18
ATOM	1 599	CB	MET		-1.967 -1.370				31.53
ATOM	600	CG	MET						35.11
ATOM	601	SD	MET		-2.377			1.00	42.40
ATOM		CE	MET		-3.657			1.00	50.10
ATOM		C_	MET		-3.069		-0.972	1.00	50.20
ATOM	604	0	MET		-0.976		3.572	1.00	30.86
ATOM	605	N	ILE		-1.218	-3.425	3.210	1.00	30.07
ATOM		CA	ILE		0.119		4.259	1.00	30.92
ATOM	608	CB	ILE	1538	1.173	-2.923	4.563	1.00	28.12
ATOM	609	CG2	ILE	1538	2.359	-2.254	5.313	1.00	28.71
ATOM	610	CG1	ILE	1538	3.310	-3.303	5.865	1.00	29.72
ATOM	611	CD1	ILE	1538	3.126	-1.343	4.350	1.00	30.79
ATOM	612	C	ILE	1538	4.375	-0.745	4.945	1.00	32.46
ATOM	613	ō	ILE	1538	0.717	-4.179	5.299	1.00	26.33
MOTA	614	N	GLY	1538	1.178	-5.276	4.996	1.00	24.20
ATOM	616	CA	GLY	1539	-0.188	-4.027	6.258	1.00	27.41
MOTA	617	C	GLY	1539	-0.651	-5.190	6.997	1.00	27.83
ATOM	618	Ö	GLY	1539	0.240	-5.533	8.179	1.00	29.10
MOTA	619	N	LYS	1540	1.308	-4.937	8.368	1.00	30.33
ATOM	621	CA	LYS	1540	-0.157	-6.561	8.916	1.00	29.46
ATOM	622	CB	LYS	1540	0.539	-6.976	10.120	1.00	29.27
ATOM	623	ĊG	LYS	1540	-0.470	-7.520	11.139	1.00	27.01
ATOM	624	CD	LYS	1540	-1.438	-6.483	11.638	1.00	29.58
ATOM	625	CE	LYS	1540	-2.496	-7.103	12.530	1.00	39.41
ATOM	626	NZ	LYS	1540	-3.548	-6.069	12.952	1.00	44.14
ATOM	630	C	LYS	1540	-2.994	-4.996	13.828	1.00	46.92
ATOM	631	ō	LYS	1540	1.679	-7.962	10.020	1.00	27.17
MOTA	632	N	HIS	1541	1.745	-8.794	9.111	1.00	26.20
ATOM	634	CA	HIS	1541	2.565	-7.856	11.006	1.00	26.96
ATOM	635	CB	HIS	1541	3.690	-8.761	11.144	1.00	27.30
ATOM	636	CG	HIS		4.787	-8.506	10.120	1.00	22.20
ATOM	637	CD2	HIS	1541	5.849	-9.555	10.125	1.00	21.32
ATOM	638	ND1	HIS	1541	5.886	-10.789	9.555	1.00	23.29
ATOM	640	CE1	HIS	1541	7.052	-9.413	10.791	1.00	19.41
ATOM	641	NE2	HIS	1541	7.775	-10.509	10.633	1.00	23.61
ATOM	643	C	HIS	1541	7.097	-11.355	9.889	1.00	21.81
ATOM	644	0		1541	4.245	-8.640	12.565		28.64
ATOM	645	N	HIS	1541	4.290	-7.549	13.132		30.64
ATOM	647		LYS	1542	4.650	-9.791	13.108		29.47
ATOM	648	CA CB	LYS	1542	5.200	-9.893		_	28.78
ATOM	649	CG	LYS	1542	5.683	-11.326			30.16
ATOM	650		LYS	1542	6.232	-11.572			32.63
ATOM	651	CD	LYS	1542	5.277	-11.046			42.90
•		CE	LYS	1542	5.659				48.13

ATOM	652	NZ	LYS	1542	4.726	-10.930	19.564	1.00	54.87
ATOM	656	С	LYS	1542	6.351	-8.928	14.705	1.00	26.54
MOTA	657	0	LYS	1542	6.440	-8.321	15.773	1.00	26.19
ATOM	658	N	ASN	1543	7.193	-8.733	13.697	1.00	24.36
ATOM	660	CA	ASN	1543	8.357	-7.874	13.852	1.00	24.08
ATOM	661	CB	ASN	1543	9.601	-8.596	13.359	1.00	22.69
ATOM	662	CG	ASN	1543	9.781	-9.950	14.029	1.00	22.81
MOTA	663	OD1	ASN	1543	9.664	-10.996	13.388	1.00	23.62
MOTA	664	ND2	ASN	1543	10.028	-9.938	15.324	1.00	24.94
MOTA	667	C	ASN	1543	8.318	-6.429	13.377	1.00	23.48
ATOM	668	0	ASN	1543	9.351	-5.861	13.059	1.00	22.94
ATOM	669	N	ILE	1544	7.130	-5.821	13.380	1.00	24.15
MOTA	671	CA	ILE	1544	6.976	-4.407	13.012	1.00	24.60
ATOM	672	CB	ILE	1544	6.516	-4.191	11.531	1.00	24.90
ATOM	673	CG2	ILE	1544	7.495	-4.852	10.571	1.00	21.57
MOTA	674	CG1	ILE	1544	5.081	-4.688	11.316	1.00	26.66
MOTA	675	CD1	ILE	1544	4.481	-4.321	9.945	1.00	23.98
MOTA	676	C	ILE	1544	5.954	-3.785	13.955	1.00	24.78
MOTA	677	0	ILE	1544	5.160	-4.503	14.558	1.00	27.87
MOTA	678	N	ILE	1545	6.035	-2.474	14.159	1.00	26.39
ATOM	680	CA	ILE	1545	5.089	-1.779	15.025	1.00	26.79
MOTA	681	CB	ILE	1545	5.588	-0.345	15.384	1.00	28.85
ATOM	682	CG2	ILE	1545	4.512	0.449	16.103	1.00	23.60
MOTA	683	CG1	ILE	1545	6.833	-0.423	16.269	1.00	27.20
MOTA	684	CD1	ILE	1545	6.565	-0.990	17.639	1.00	27.12
MOTA	685	С	ILE	1545	3.792	-1.708	14.224	1.00	26.99
ATOM	686	0	ILE	1545	3.720	-1.023	13.197	1.00	27.61
ATOM	687	N	ASN	1546	2.809	-2.495	14.654	1.00	26.70
ATOM	689	CA	ASN	1546	1.514	-2.565	13.983	1.00	26.53
ATOM	690	CB	ASN	1546	0.871	-3.953	14.169	1.00	26.23
ATOM	691	CG	ASN	1546	1.695	-5.072	13.551	1.00	24.96
MOTA	692	OD1	ASN	1546	1.773	-5.206	12.330	1.00	28.08
MOTA	693	ND2	ASN	1546	2.319	-5.872	14.387	1.00	22.38
ATOM	696	, C	ASN	1546	0.521	-1.497	14.418	1.00	26.89
MOTA	697	0	ASN	1546	0.610	-0.952	15.523	1.00	27.40
MOTA	698	N	LEU	1547	-0.349	-1.138	13.481	1.00	27.77
ATOM	700	CA	LEU	1547	-1.416	-0.175	13.701	1.00	28.28
MOTA	701	CB	LEU	1547	-1.958	0.313	12.361	1.00	27.04
MOTA	702	CG	LEU	1547	-3.199	1.194	12.408	1.00	25.74
MOTA	703	CD1	LEU	1547	-2.836	2.575	12.950	1.00	27.66
MOTA	704	CD2	LEU	1547	-3.799	1.289	11.014	1.00	23.38
MOTA	705	С	LEU	1547	-2.498	-0.972	14.435	1.00	29.80
MOTA	706	0	LEU	1547	-2.766	-2.135	14.105	1.00	28.63
ATOM	707	N	LEU	1548	-3.088	-0.351	15.448	1.00	29.91
ATOM	709	CA	LEU	1548	-4.114	-0.997	16.256	1.00	28.46
MOTA	710	СВ	LEU	1548	-3.735	-0.956	17.749	1.00	26.76
MOTA	711	CG	LEU	1548	-2.460	-1.701	18.162	1.00	22.44
ATOM	712	CD1	LEU	1548	-2.277	-1.554	19.653	1.00	21.91
ATOM	713	CD2	LEU	1548	-2.551	-3.179	17.778	1.00	20.79
ATOM	714	c	LEU	1548	-5.480	-0.365	16.058	1.00	27.31
ATOM	715	ō	LEU	1548	-6.489	-1.043	16.193	1.00	28.25
ATOM	716	N	GLY	1549	-5.506	0.925	15.732	1.00	24.02
ATOM	718	CA	GLY	1549	-6.774	1.598	15.553	1.00	24.57
ATOM	719	C	GLY	1549	-6.548	3.077	15.395	1.00	25.19
		_		ムフマフ	5.540	3.077	<b>エン・</b> フラフ	±. ∪∪	CJ. LJ

3 500									
ATON		0	GLY		-5.400	3.488	15.231	1.00	28.77
ATON		N	ALA	· -	-7.617	3.875	15.427	1.00	
ATON MOTA		CA	ALA		-7.487	5.319	15.282	1.00	
ATOM			ALA		-7.206	5.680		1.00	
ATOM		C	ALA		-8.695	6.103	15.765	1.00	23.95
ATOM		0	ALA		-9.810	5.590	15.780	1.00	24.95
ATOM		И	CYS		-8.444	7.336	16.199	1.00	25.03
ATOM		CA	CYS		-9.482	8.270	16.639	1.00	28.21
ATOM		CB	CYS		-9.221	8.774	18.055	1.00	26.76
ATOM		SG	CYS	_	-9.378	7.521	19.317	1.00	34.39
ATOM		C	CYS		-9.359	9.426	15.656	1.00	29.98
ATOM		O N	CYS		-8.482	10.281		1.00	32.14
ATOM		N CA	THR	1552	-10.198	9.412	14.625	1.00	31.09
ATOM		CB	THR	1552	-10.135	10.435	13.595	1.00	32.91
ATOM		OG1	THR THR	1552	-10.052	9.781	12.189	1.00	32.60
ATOM		CG2	THR	1552	-11.276	9.097	11.890	1.00	32.12
ATOM	741	C	THR	1552 1552	-8.928	8.768	12.144	1.00	32.74
ATOM	742	Ö	THR	1552	-11.282	11.419	13.591	1.00	35.26
ATOM	743	N	GLN	1553	-11.171	12.525	13.057	1.00	35.10
ATOM	745	CA	GLN	1553	-12.397 -13. <b>58</b> 5	11.014	14.179	1.00	39.01
ATOM	746	СВ	GLN	1553	-13.383	11.846	14.180	1.00	41.97
ATOM	747	CG	GLN	1553	-14.832	10.968	14.020	1.00	41.17
ATOM	748	CD	GLN	1553	-14.915	10.238	12.672	1.00	39.06
ATOM	749	OE1	GLN	1553	-15.785	11.200 12.045	11.496	1.00	41.84
ATOM	750	NE2	GLN	1553	-13.876	11.090	11.359	1.00	41.92
ATOM	753	C	GLN	1553	-13.727	12.777	10.652 15.372	1.00	42.33
ATOM	754	0	GLN	1553	-13.358	12.423	16.489	1.00	45.35
ATOM	755	N	ASP	1554	-14.225	13.981	15.090	1.00	47.02
ATOM	757	CA	ASP	1554	-14.479	15.016	16.084	1.00 1.00	48.60
MOTA	758	CB	ASP	1554	-15.832	14.766	16.758	1.00	50.64
ATOM	759	CG	ASP	1554	-17.003	14.955	15.809	1.00	54.52 60.54
ATOM	760	OD1	ASP	1554	-18.072	15.409	16.274	1.00	66.04
ATOM	761	OD2	ASP	1554	-16.860	14.661	14.601	1.00	65.09
ATOM	762	C	ASP	1554	-13.395	15.173	17.133	1.00	49.89
ATOM	763	0	ASP	1554	-13.611	14.879	18.310	1.00	51.48
ATOM	764	N	GLY	1555	-12.232	15.643	16.699	1.00	48.40
ATOM	766	CA	GLY	1555	-11.131	15.834	17.617	1.00	46.16
ATOM	767	C	GLY	1555	-9.798	15.626	16.935	1.00	44.64
ATOM	768	0	GLY	1555	-9.737	15.581	15.716	1.00	45.22
ATOM ATOM	769	N	PRO	1556	-8.708	15.525	17.702	1.00	44.68
ATOM	770 771	CD	PRO	1556	-8.672	15.683	19.164	1.00	45.39
ATOM	771 772	CA	PRO	1556	-7.359	15.326	17.177	1.00	42.95
ATOM	773	CB	PRO	1556	-6.484	15.549	18.411	1.00	43.74
ATOM	774	CG C	PRO	1556	-7.354	16.347	19.345	1.00	47.32
ATOM	775		PRO	1556	-7.164	13.912	16.665	1.00	42.34
ATOM		0	PRO	1556	-7.636	12.953	17.287	1.00	42.75
ATOM	776 778	N	LEU	1557	-6.451	13.788	15.547	1.00	39.83
ATOM	778 779	CA CB	LEU	1557	-6.169	12.490	14.954	1.00	36.64
ATOM	780		LEU	1557	-5.496	12.669	13.587	1.00	34.49
ATOM	781	CG CD1	LEU	1557	-5.009	11.404	12.870	1.00	31.29
ATOM	782	CD2	LEU	1557	-6.169	10.436	12.628	1.00	27.86
ATOM	783	CD2	LEU	1557 1557	-4.314	11.775	11.570	1.00	25.40
	-	_			-5.244	11.732	15.894	1.00	35.44





MOTA	784	0	LEU	1557	-4.210	12.264	16.316	1.00	36.12
MOTA	785	N	TYR	1558	-5.664	10.539	16.292	1.00	32.49
ATOM	787	CA	TYR	1558	-4.861	9.697	17.157	1.00	31.87
MOTA	788	CB	TYR	1558	-5.590	9.348	18.470	1.00	33.93
MOTA	789	CG	TYR	1558	-5.695	10.476	19.471	1.00	35.34
ATOM	790	CD1	TYR	1558	-6.566	10.394	20.565	1.00	37.12
ATOM	791	CE1	TYR	1558	-6.683	11.456	21.479	1.00	36.44
ATOM	792	CD2	TYR	1558	-4.945	11.636	19.317	1.00	37.27
MOTA	793	CE2	TYR	1558	-5.054	12.690	20.213	1.00	39.62
ATOM	794	CZ	TYR	1558	-5.921	12.598	21.289	1.00	40.05
MOTA	795	OH	TYR	1558	-6.008	13.668	22.155	1.00	44.98
ATOM	797	C	TYR	1558	-4.600	8.419	16.387	1.00	31.58
ATOM	798	0	TYR	1558	-5.532	7.750	15.936	1.00	30.22
ATOM	799	N	VAL	1559	-3.331	8.129	16.153	1.00	33.43
ATOM	801	CA	VAL	1559	-2.947	6.907	15.463	1.00	31.42
ATOM	802	CB	VAL	1559	-1.849	7.160	14.419	1.00	32.31
ATOM	803	CG1	VAL	1559	-1.516	5.851	13.675	1.00	26.79
ATOM	804	CG2	VAL	1559	-2.308	8.265	13.453	1.00	30.63
MOTA	805	С	VAL	1559	-2.438	5.979	16.556	1.00	28.67
MOTA	806	0	VAL	1559	-1.393	6.223	17.155	1.00	30.08
ATOM	807	N	ILE	1560	-3.230	4.960	16.852	1.00	25.80
ATOM	809	CA	ILE	1560	-2.915	3.998	17.894	1.00	25.33
ATOM	810	CB	ILE	1560	-4.219	3.443	18.506	1.00	22.34
ATOM	811	CG2	ILE	1560	-3.931	2.695	19.784	1.00	20.36
ATOM	812	CG1	ILE	1560	-5.172	4.603	18.809	1.00	21.34
ATOM	813	CD1	ILE	1560	-6.583	4.190	19.093	1.00	20.68
ATOM	814	С	ILE	1560	-2.073	2.857	17.341	1.00	27.16
ATOM	815	0	ILE	1560	-2.520	2.116	16.455	1.00	29.67
ATOM	816	N	VAL	1561	0.858	2.714	17.860	1.00	27.69
ATOM	818	CA	VAL	1561	0.060	1.667	17.411	1.00	28.27
ATOM	819	CB	VAL	1561	1.311	2.269	16.696	1.00	27.34
ATOM	820	CG1	VAL	1561	0.892	3.019	15.445	1.00	21.76
ATOM	821	CG2	VAL	1561	2.074	3.201	17.639	1.00	26.00
ATOM	822	С	VAL	1561	0.509	0.809	18.588	1.00	28.70
ATOM	823	0	VAL	1561	0.221	1.139	19.746	1.00	30.52
ATOM	824	N	GLU	1562	1.166	-0.311	18.286	1.00	28.64
ATOM	826	CA	GLU	1562	1.658	-1.220	19.318	1.00	27.77
ATOM	827	CB	GLU	1562	2.278	-2.465	18.693	1.00	24.57
ATOM	828	CG	GLU	1562	1.251	-3.452	18.208	1.00	24.76
ATOM	829	CD	GLU	1562	1.864	-4.641	17.501	1.00	27.27
ATOM	830	OE1	GLU	1562	1.272	-5.739	17.580	1.00	28.27
ATOM	831	OE2	GLU	1562	2.920	-4.487	16.849	1.00	29.25
MOTA	832	C	GLU	1562	2.674	-0.538	20.217	1.00	28.79
ATOM	833	0	GLU	1562	3.453	0.292	19.760	1.00	29.38
ATOM	834	N	TYR	1563	2.627	-0.871	21.503	1.00	30.84
MOTA	836	CA	TYR	1563	3.534	-0.304	22.493	1.00	31.43
ATOM	837	CB	TYR	1563	2.782	-0.088	23.799	1.00	32.10
ATOM	838	CG	TYR	1563	3.632	0.376	24.952	1.00	33.93
MOTA	839	CD1	TYR	1563	4.366	1.552	24.873	1.00	34.85
MOTA	840	CE1	TYR	1563	5.140	1.992	25.947	1.00	37.53
MOTA	841	CD2	TYR	1563	3.683	~0.356	26.136	1.00	34.81
ATOM	842	CE2	TYR	1563	4.452	0.072	27.211	1.00	34.01
ATOM	843	CZ	TYR	1563	5.173	1.245	27.113	1.00	35.79
ATOM	844	ОН	TYR	1563	5.920	1.677	28.184	1.00	39.10

		846	C	Т	YR 15	63 4	767					
		847	0		YR 15		.767	-1.1			.00	31.38
AT	OM	848	N		LA 156		672	-2.3		905 1	.00	30.73
AT	OM .	850	CA		LA 156		930	-0.5			.00	32.23
AT		851	CB		LA 156	-	198	-1.2	_		00	35.90
ATO		352	С		LA 156		178	-0.8		33 1.	00	36.44
AT		353	0		LA 156		711	-0.7			00	36.52
ATO	3 MC	354	N	SE		- •	332	0.34		03 1.	00	39.16
ATO	OM 8	156	CA	SE			424	-1.48				34.62
ATC	ом в	57	СВ	SE			801	-1.07		00 1.		34.91
ATC	8 MC	58	OG	SE		•	124	-1.94				32.11
ATO	-	60	C	SE			506	-3.27				32.92
ATO	8 M	61	0	SE				-0.96		96 1.		35.56
ATO	м в	62	N	LY				-0.21		36 1.0		38.69
ATO	M 8	64	CA	LY	•			-1.67	3 26.24			33.70
ATO	M 8	65	CB	LY				-1.62	5 26.52			31.40
ATO	M 86	56	CG	LYS				-3.03	3 26.53			0.56
ATO		57	CD	LYS		_		-3.869	27.66		_	2.32
ATO	4 86	8	CE	LYS		>		-5.308	27.59			6.47
ATOM	1 86	9	NZ	LYS		_		-6.031	28.87			6.97
ATOM	1 87	'3	C	LYS				-7.436	28.80			1.62
ATOM	1 87	4	0	LYS				-0.664	25.68			2.18
ATOM			N	GLY				-0.691	25.71		_	2.57
ATOM	87	7	CA	GLY				0.223				3.39
ATOM	87		C	GLY		12.34		1.224		1.0		2.13
ATOM	87		o	GLY	•	13.07		0.719	22.928			L.70
ATOM			N	ASN		12.91		-0.430	22.530			3.30
ATOM			CA	ASN		13.88		1.589	22.331			38
ATOM			CB	ASN	1568	14.63		1.230	21.139			.,00
ATOM	884		CG	ASN	1568	15.06		2.478	20.365			.30
ATOM	889	_	DD1	ASN	1568	16.12	7	3.271	21.074			.47
ATOM	886		VD2	ASN	1568	17.13		2.733	21.508			. 19
ATOM	889			ASN	1568	15.93		4.580	21.144	1.00		.13
ATOM	890			ASN	1568	15.80		0.295	21.393	1.00		.62
ATOM	891			LEU	1568	16.35		0.256	22.483	1.00		. 91
ATOM	893		'A	LEU	1569	16.193		-0.428	20.354	1.00		. 92
ATOM	894	_	В	LEU	1569	17.269		-1.403	20.417	1.00	31	
ATOM	895		G	LEU	1569	17.418		-2.083	19.054	1.00	29.	
ATOM	896		D1	LEU	1569 1569	18.415		-3.231	18.893	1.00	29.	
ATOM	897		D2	LEU		18.284		-4.261	20.024	1.00	21.	
ATOM	898	C		LEU	1569	18.184		-3.863	17.523	1.00	24.	
ATOM	899	o		LEU	1569	18.609		0.838	20.878	1.00	32.	
ATOM	900	N		ARG	1569	19.328		1.499	21.618	1.00	33.	
ATOM	902	CZ		ARG	1570	18.954		0.370	20.432	1.00	33.	
ATOM	903	CI		ARG	1570	20.218		0.983	20.834	1.00	33.	
ATOM	904	CC		ARG	1570	20.348		2.394	20.256	1.00	32.	
ATOM	905	CI	_		1570	21.586		3.129	20.758	1.00	38.	30 30
ATOM	906	NE		ARG	1570	21.672		4.538	20.221	1.00	41.	
ATOM	908	CZ		ARG	1570	20.428		5.278	20.412	1.00		
ATOM	909			ARG	1570	19.975		5.721	21.584	1.00	49.8	
ATOM	912	NH		ARG	1570	20.659		5.510	22.712	1.00	52.3	
ATOM	915	NH		ARG	1570	18.824		6.377	21.622	1.00	51.6	
ATOM	916	C			1570	20.308			22.371	1.00	53.2	
ATOM	917	0			1570	21.184			22.970	1.00	33.9	
	J + /	N	G	LU	1571	19.359			22.981	1.00	33.1	
SSSD/551	145 00	١1								1.00	33.4	5
	マン・ソし	<i>,</i> (										

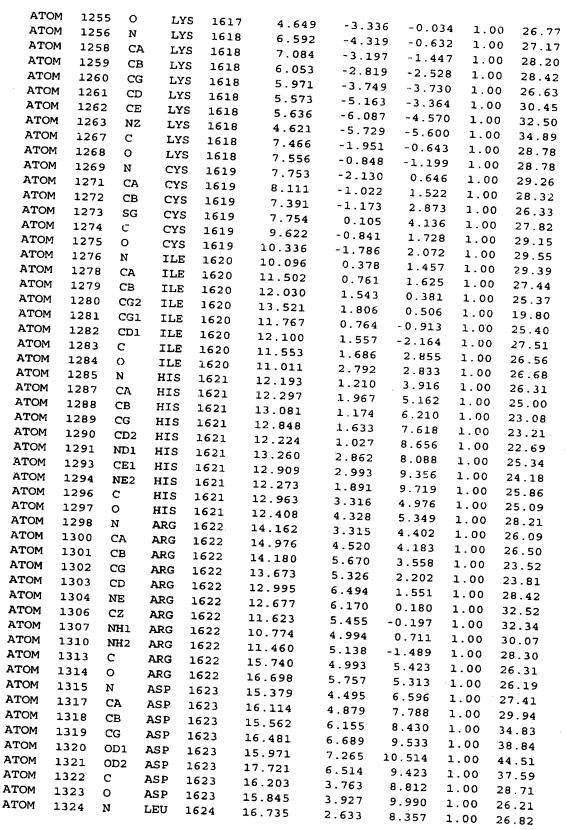
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MOTA	921	CG	GLU	1571	18.158	4.145	24.354	1.00	41.61
MOTA	922	CD	GLU	1571	16.814	4.870	24.318	1.00	47.33
ATOM	923	OEl	GLU	1571	15.759	4.199	24.362	1.00	50.68
ATOM	924	OE2	GLU	1571	16.812	6.120	24.218	1.00	48.07
MOTA	925	С	GLU	1571	19.223	0.487	25.098	1.00	34.39
MOTA	926	0	GLU	1571	19.968	0.202	26.041	1.00	34.04
MOTA	927	N	TYR	1572	18.363	-0.376	24.5 <b>72</b>	1.00	33.49
MOTA	929	CA	TYR	1572	18.204	-1.728	25.083	1.00	30.45
MOTA	930	CB	TYR	1572	17.210	-2.495	24.202	1.00	28.13
ATOM	931	CG	TYR	1572	17.074	-3.971	24.487	1.00	25.80
MOTA	932	CD1	TYR	1572	16.105	-4.443	25.371	1.00	28.92
ATOM	933	CE1	TYR	1572	15.954	-5.804	25.618	1.00	30.03
ATOM	934	CD2	TYR	1572	17.899	-4.899	23.863	1.00	24.61
MOTA	935	CE2	TYR	1572	17.760	-6.260	24.102	1.00	26.05
MOTA	936	CZ	TYR	1572	16.790	-6.705	24.982	1.00	29.23
ATOM	937	OH	TYR	1572	16.651	-8.052	25.227	1.00	33.74
ATOM	939	С	TYR	1572	19.549	-2.447	25.113	1.00	31.30
MOTA	940	0	TYR	1572	19.880	-3.126	26.090	1.00	32.43
MOTA	941	N	LEU	1573	20.334	-2.266	24.058	1.00	29.68
MOTA	943	CA	LEU	1573	21.625	-2.923	23.972	1.00	30.04
ATOM	944	CB	LEU	1573	22.145	-2.909	22.529	1.00	26.13
MOTA	945	CG	LEU	1573	21.532	-3.870	21.490	1.00	25.24
MOTA	946	CD1	LEU	1573	22.097	-3.563	20.113	1.00	19.70
MOTA	947	CD2	LEU	1573	21.807	-5.317	21.839	1.00	22.05
MOTA	948	C	LEU	1573	22.645	-2.308	24.927	1.00	34.47
MOTA	949	0	LEU	1573	23.354	-3.031	25.644	1.00	34.95
MOTA	950	N	GLN	1574	22.691	-0.980	24.978	1.00	35.47
MOTA	952	CA	GLN	1574	23.639	-0.293	25.850	1.00	37.09
MOTA	953	CB	GLN	1574	23.601	1.206	25.579	1.00	36.70
ATOM	954	CG	GLN	1574	24.033	1.559	24.171	1.00	39.77
ATOM	955	CD	GLN	1574	23.960	3.045	23.884	1.00	41.51
ATOM	956	OE1	GLN	1574	23.592	3.837	24.751	1.00	42.57
ATOM	957	NE2	GLN	1574	24.288	3.431	22.652	1.00	41.34
MOTA	960	C	GLN	1574	23.400	-0.588	27.332	1.00	37.85
ATOM	961	0	GLN	1574	24.343	-0.801	28.090	1.00	38.87
ATOM	962	N ·	ALA	1575	22.131	-0.667	27.720	1.00	39.01
ATOM	964	CA	ALA	1575	21.740	-0.944	29.098	1.00	37.00
MOTA MOTA	965	CB	ALA	1575	20.261	-0.678	29.273	1.00	35.71
	966	C	ALA	1575	22.061	-2.359	29.559	1.00	39.14
ATOM	967 969	O N	ALA	1575	21.839	-2.692	30.719	1.00	43.81
ATOM	968	N	ARG	1576	22.563	-3.201	28.665	1.00	38.39
ATOM ATOM	970 971	CA CB	ARG	1576	22.897	-4.568	29.032	1.00	37.71
MOTA	972	CG	ARG ARG	1576	21.994	-5.544	28.290	1.00	38.26
				1576	20.555	-5.383	28.700	1.00	38.00
ATOM	973	CD	ARG	1576	19.653	-6.282	27.920	1.00	34.74
ATOM	974 976	NE C7	ARG	1576 1576	18.279	-6.190 -5.066	28.388	1.00	32.88
ATOM ATOM	976 977	CZ	ARG	1576	17.572	-5.066	28.442	1.00	34.02
ATOM	977 980	NH1	ARG	1576	18.114	-3.913	28.068	1.00	35.57
ATOM	980 983	NH2 C	ARG	1576	16.298	-5.102 -4.933	28.800	1.00	36.71
ATOM	983 984	0	ARG ARG	1576	24.365	-4.927 -6.112	28.828	1.00	39.59
ATOM	985	N	ARG	1576	24.735	-6.113	28.788	1.00	39.83
AION	203	14	MKG	1577	25.200	-3.900	28.687	1.00	38.82

ATO	98 MC	7 CA	AR	G 1577	26.63	14 10	1 00	_	
ATO		в св							39.07
ATC		9 CG	AR			_			34.91
ATC		CD	ARC			_			33.87
ATC	M 991	NE	ARC		27.72				33.06
ATO		CZ	ARG		28.17		<del>-</del>		38.87
ATO	M 994	NH			28.68	_		_	39.76
ATO	M 997	NH2	2 ARG		28.12	_			40.68
ATO	M 100	0 C	ARG		27.18:				43.26
ATO		1 0	ARG		26.586				41.58
ATO	M 100	2 N	PRO		28.294				42.48
ATO			PRO		29.110				43.07
ATO		4 CA	PRO		28.839			1.00	43.36
ATO		5 CB	PRO		29.966		31.223	1.00	42.69
ATO	_	6 CG	PRO	1578	30.412		30.857	1.00	42.22
ATON		7 C	PRO	1578	29.366		29.516	1.00	43.64
ATOM		3 0	PRO	1578	29.530		31.882	1.00	43.37
ATOM		9 N	PRO	1579	29.596		31.215	1.00	42.50
ATOM		CD C	PRO	1579	29.279		33.198	1.00	45.24
ATOM		CA	PRO	1579	30.099		34.174	1.00	44.69
ATOM			PRO	1579	29.979		33.882	1.00	46.27
ATOM			PRO	1579	28.894		35.353	1.00	45.78
ATOM		-	PRO	1579	31.548	-2.869	35.361	1.00	46.15
ATOM			PRO	1579	32.410	-3.753	33.500	1.00	48.38
ATOM			GLU	1592	19.022	-5.398	33.478	1.00	50.64
ATOM			GLU	1592	20.442	-5.048	32.495 32.492	1.00	65.98
ATOM			GLU	592ء	20.796	-4.241	33.740	1.00	64.80
ATOM	1020	_	GLU	1592	21.351	-6.275	32.371	1.00	67.30
ATOM	1021	0	GLU	1592	22.545	-6.149	32.089	1.00 1.00	63.80
ATOM	1022	N	GLU	1593	20.789	-7.458	32.607		65.21
ATOM ATOM	1024	CA	GLU	1593	21.560	-8.691	32.495		61.44
ATOM	1025	CB	GLU	1593	20.681	-9.899	32.807		60.82
ATOM	1026	C	GLU	1593	22.144	-8.803	31.089		51.47
ATOM	1027	0	GLU	1593	21.468	-8.525	30.097	_	59.12 59.49
ATOM	1028	N	GLN	1594	23.408	-9.201	31.017		57. <b>3</b> 3
ATOM	1030 1031	CA	GLN	1594	24.103	-9.334	29 744		55.30
ATOM	1031	CB	GLN	1594	25.523	- 9.880	29.957		54.87
ATOM	1032	CD CD	GLN	1594	26.438	-8. <b>9</b> 59	30.757		53.34
ATOM	1034		GLN	1594	27.704	-9.660			55.27
ATOM	1035	OE1 NE2	GLN	1594	28.256	-10.536			66.47
ATOM	1033	C C	GLN	1594	28.166	-9.275			1.46
ATOM	1038	0	GLN	1594	23.336	-10.229			2.29
ATOM	1040	N	GLN	1594	22.648	-11.166			2.56
ATOM	1042	CA		1595	23.447	-9.913			9.40
ATOM	1043			1595	22.783	-10.676			6.00
ATOM	1044			1595	22.452	-9.760			2.94
ATOM	1045			1595	21.390	-8.711			3.90
ATOM	1046		_	1595	21.495				9.46
ATOM	1047			1595	20.005	-9.347			1.86
ATOM	1048			1595	23.741			_	3.96
ATOM	1049			1595	24.950	-11.550			4.24
ATOM	1051			1596	23.217	-12.941			3.29
ATOM	1052			1596	24.076		25. <b>275</b> 1		2.40
			JER .	1596	23.388	-15.374			1.83
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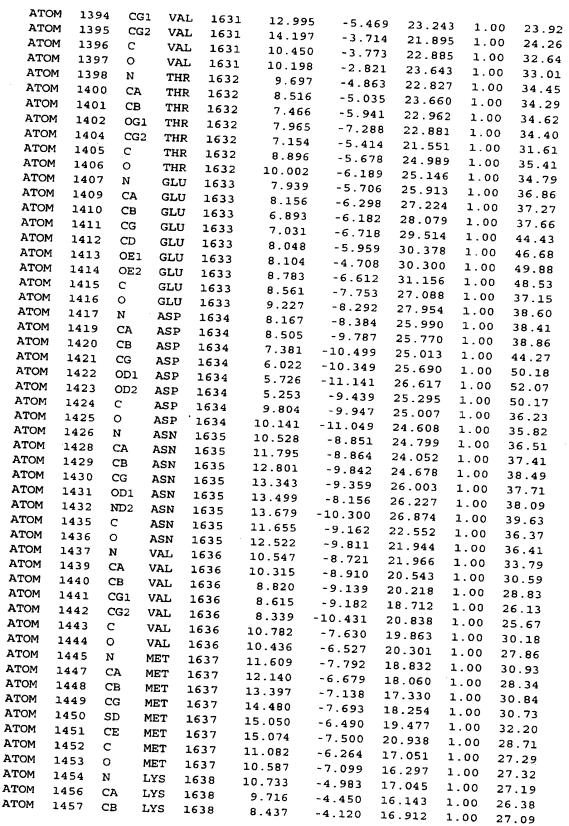
MOTA	1 1053	OG	SER	1596	22.218	-15.483	24.697	1.00	44.25	
ATOM	1 (1055	С	SER	1596	24.392	-13.817	23.800	1.00	42.64	
ATOM	1 1056	0	SER	1596	23.857	-12.900	23.171	1.00	43.14	
MOTA	1 1057	N	SER	1597	25.277	-14.645	23.255	1.00	42.59	
ATOM	1 1059	CA	SER	1597	25.629	-14.553	21.850	1.00	42.91	
ATOM	1060	CB	SER	1597	26.739	-15.547	21.516	1.00	45.26	
ATOM	1 1061	OG	SER	1597	27.812	-15.436	22.431	1.00	56.41	
MOTA	1 1063	С	SER	1597	24.380	-14.909	21.048	1.00	42.35	
ATOM	1 1064	0	SER	1597	24.113	-14.322	20.003	1.00	43.71	
ATOM	1 1065	N	LYS	1598	23.621	-15.881	21.544	1.00	40.61	
MOTA	1 1067	CA	LYS	1598	22.405	-16.298	20.867	1.00	38.61	
ATOM	1 1068	CB	LYS	1598	21.848	-17.575	21.483	1.00	36.33	
ATOM	1069	CG	LYS	1598	21.135	-18.439	20.468	1.00	40.09	
ATOM	1070	CD	LYS	1598	20.213	-19.434	21.118	1.00	43.39	
ATOM	1071	CE	LYS	159B	19.766	-20.494	20.122	1.00	48.25	
ATOM	1072	NZ	LYS	1598	20.930	-21.290	19.623	1.00	50.46	
ATOM	1076	C	LYS	1598	21.348	-15.194	20.895	1.00	38.17	
ATOM	1077	О	LYS	1598	20.579	-15.053	19.945	1.00	41.27	
MOTA	1078	N	ASP	15 <b>9</b> 9	21.321	-14.408	21.969	1.00	35.90	
ATOM	1080	CA	ASP	1599	20.366	-13.307	22.099	1.00	34.08	
ATOM	1081	CB	ASP	1599	20.450	-12.661	23.477	1.00	37.83	
ATOM	1082	CG	ASP	1599	19.822	-13.505	24.562	1.00	39.93	
ATOM	1083	OD1	ASP	1599	20.089	-13.217	25.742	1.00	45.85	
ATOM	1084	OD2	ASP	1599	19.060	-14.444	24.240	1.00	41.06	
ATOM	1085	C	ASP	1599	20.634	-12.243	21.061	1.00	32.37	
ATOM	1086	0	ASP	1599	19.704	-11.701	20.466	1.00	32.58	
ATOM	1087	N	LEU	1600	21.915	-11.945	20.873	1.00	30.45	
ATOM	1089	CA	LEU	1600	22.355	-10.948	19.902	1.00	29.59	
ATOM	1090	CB	LEU	1600	23.841	-10.654	20.097	1.00	28.59	
ATOM	1091	CG	LEU	1600	24.238	-10.057	21.449	1.00	24.59	
ATOM		CD1	LEU	1600	25.747	-9.869	21.522	1.00	18.40	
ATOM	1093	CD2	LEU	1600	23.529	-8.745	21.626	1.00	21.71	
ATOM		C,	LEU	1600	22.073	-11.393	18.458	1.00	28.54	
ATOM		O	LEU	1600	21.578	-10.613	17.648	1.00	25.59	
ATOM		N	VAL	1601	22.377	-12.645	18.134	1.00	29.13	
ATOM		CA	VAL	1601	22.111	-13.154	16.793	1.00	29.74	
MOTA		CB	VAL	1601	22.780	-14.513	16.551	1.00	29.63	
ATOM		CG1	VAL	1601	22.615	-14.922	15.105	1.00	29.30	
ATOM		CG2	VAL	1601	24.259	-14.422	16.873	1.00	28.52	
ATOM		C	VAL	1601	20.591	-13.247	16.564	1.00	29.98	
ATOM		0	VAL	1601	20.106	-13.040	15.452	1.00	29.73	
ATOM		N	SER	1602	19.855	-13.493	17.645	1.00	30.97	
ATOM		CA	SER	1602	18.399	-13.576	17.607	1.00	29.64	
ATOM		CB	SER	1602	17.894	-14.141	18.925	1.00	30.45	
MOTA		OG	SER	1602	16.483	-14.158	18.962	1.00	39.63	
ATOM		C	SER	1602	17.784	-12.192	17.343	1.00	29.30	
ATOM		0	SER	1602	16.772	-12.071	16.641	1.00	28.74	
MOTA		N	CYS	1603	18.385	-11.157	17.925	1.00	27.68	
MOTA		CA	CYS	1603	17.931	-9.783	17.717	1.00	27.32	
MOTA		CB	CYS	1603	18.791	-8.790	18.516	1.00	25.40	
ATOM		SG	CYS	1603	18.472	-7.039	18.177	0.50		PRT1
MOTA		С	CYS	1603	18.057	-9.468	16.225	1.00	28.34	
ATOM		0	CYS	1603	17.134	-8. <del>9</del> 26	15.629	1.00	29.70	
ATOM	1119	N	ALA	1604	19.192	-9.837	15.627	1.00	29.36	

ATO	OM 11:	21 C	A AL	A 1604	10	_			
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ATO:					17.179				
ATO					17.107		13.488		28.74
ATO					16.018		12.912		31.12
ATO					16.152	-0.230	11.650	1.00	32.53
ATO					15.144		11.121		30.84
ATON					14.853		13.634	1.00	31.21
ATON			2 TYF TYF		13.850		13.116	1.00	29.69
ATON			TYR		14.002	-16.296	11.864	1.00	30.82
ATOM					12.990	-17.069	11.359	1.00	33.77
ATOM			TYR		15.788	-11.758	12.853	1.00	27.33
ATOM			TYR		15.152	-11.691	11.805	1.00	27.94
ATOM			GLN		15.323	-11.292	14.007	1.00	27.93
ATOM			GLN		14.008	-10.659	14.115	1.00	27.20
ATOM			GLN		13.686	-10.335	15.570	1.00	26.40
ATOM			GLN		13.301	~11.556	16.402	1.00	28.12
ATOM			GLN GLN		13.114	-11.215	17.865	1.00	30.41
ATOM				1606	12.188	-10.489	18.234	1.00	34.34
ATOM	1149			1606	14.008	-11.701	18.700	1.00	31.44
ATOM	1150	_	GLN GLN	1606	13.906	-9.397	13.275	1.00	29.67
ATOM	1151	_		1606	12.884	-9.148	12.622	1.00	30.74
ATOM	1153		VAL VAL	1607	14.970	-8.602	13.281	1.00	29.59
ATOM	1154	CB		1607	14.996	-7.377	12.501	1.00	27.00
ATOM	1155	CG1	VAL	1607	16.235	-6.544	12.842	1.00	27.20
ATOM	1156	CG2	VAL VAL	1607	16.382	-5.397	11.859	1.00	28.11
ATOM	1157	C	VAL	1607	16.113	-5.996	14.266	1.00	24.79
ATOM	1158	0	VAL	1607	14.966	-7.725	11.014	1.00	28.02
ATOM	1159	N	ALA	1607	14.229	-7.108	10.241	1.00	28.28
ATOM	1161	CA	ALA	1608	15.736	-8.741	10.626	1.00	27.56
ATOM	1162	CB	ALA	1608	15.787	-9.206	9.236	1.00	27.36
ATOM	1163	C	ALA	1608	16.801	-10.339	9.095	1.00	26.25
ATOM	1164	0	ALA	1608	14.402	-9.674	8.779	1.00	28.58
ATOM	1165	N	ARG	1608	14.013	-9.446	7.624		29.11
ATOM	1167	CA	ARG	1609	13.660	-10.326	9.680	_	28.88
ATOM	1168	CB	ARG	1609 1609	12.306	-10.797	9.376	1.00	27.17
ATOM	1169	CG	ARG	1609	11.797		10.464	1.00	29.68
ATOM	1170	CD	ARG	1609	12.458		10.439		31.65
ATOM	1171	NE	ARG		11.612	-14.049	11.177		38.21
ATOM	1173	CZ	ARG	1609	10.856	-14.897	10.269		41.10
ATOM	1174	NH1	ARG	1609	10.048	-15.872	10.667		41.97
ATOM	1177	NH2	ARG	1609	9.886	-16.125	11.959		40.69
ATOM	1180	C	ARG	1609	9.411	-16.609	9.770		13.57
ATOM	1181	0	ARG	1609	11.312	-9.654	9.183	_	25.38
ATOM	1182	N	GLY	1609	10.480	-9.693			25.75
ATOM	1184	CA	GLY	1610	11.365	-8.661			24.03
ATOM	1185	C	GLY	1610	10.480	-7.517		_	1.74
ATOM	1186	0		1610	10.734	-6.864	_		3.32
ATOM	1187	N		1610	9.805	-6.540	_		3.39
ATOM	1189	CA		1611	12.016	-6.714			4.48
•			1415 T	1611	12.453	-6.125			3.13

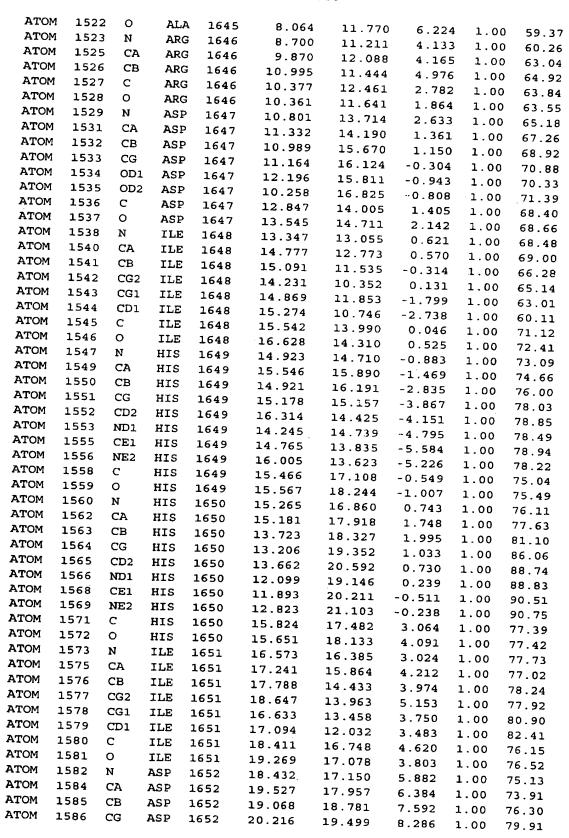
ATOM	1190	CB	MET	1611	13.949	-5.860	7.035	1.00	19.46
MOTA	1191	CG	MET	1611	14.339	-4.671	7.910	1.00	22.46
MOTA	1192	SD	MET	1611	13.457	-3.123	7.536	1.00	25.27
MOTA	1193	CE	MET	1611	13.900	-2.801	5.876	1.00	22.25
ATOM	1194	С	MET	1611	12.100	-7.005	5.811	1.00	24.87
ATOM	1195	0	MET	1611	11.699	-6.497	4.755	1.00	24.09
MOTA	1196	N	GLU	1612	12.230	-8.321	5.975	1.00	25.48
ATOM	1198	CA	GLU	1612	11.894	-9.232	4.890	1.00	25.42
ATOM	1199	CB	GLU	1612	12.155	-10.691	5.288	1.00	23.41
MOTA	1200	CG	GLU	1612	11.664	-11.679	4.232	1.00	25.14
MOTA	1201	CD	GLU	1612	11.872	-13.141	4.599	1.00	28.60
ATOM	1202	OE1	GLU	1612	11.637	-13.514	5.777	1.00	30.10
ATOM	1203	OE2	GLU	1612	12.244	-13.928	3.694	1.00	29.53
ATOM	1204	C	GLU	1612	10.418	-9.021	4.521	1.00	26.92
ATOM	1205	0	GLU	1612	10.065	-8.928	3.343	1.00	29.61
MOTA	1206	N	TYR	1613	9.576	-8.884	5.542	1.00	27.88
ATOM	1208	CA	TYR	1613	8.154	-8.675	5.337	1.00	2,3.82
ATOM	1209	СВ	TYR	1613	7.415	-8.769	6.667	1.00	24.17
ATOM	1210	CG	TYR	1613	5.941	-8.492	6.545	1.00	23.73
ATOM	1211	CD1	TYR	1613	5.064	-9.483	6.096	1.00	22.17
ATOM	1212	CE1	TYR	1613	3.698	-9.235	5.965	1.00	21.08
ATOM	1213	CD2	TYR	1613	5.419	-7.237	6.865	1.00	23.16
ATOM	1214	CE2	TYR	1613	4.054	-6.976	6.736	1.00	26.38
MOTA	1215	CZ	TYR	1613	3.200	-7.981	6.287	1.00	23.16
ATOM	1216	ОН	TYR	1613	1.855	-7.725	6.149	1.00	25.50
ATOM	1218	c	TYR	1613	7.885	-7.327	4.670	1.00	23.17
ATOM	1219	0	TYR	1613	7.147	-7.246	3.689	1.00	24.21
ATOM	1220	N	LEU	1614	8.481	-6.266	5.206	1.00	23.04
ATOM	1222	CA	LEU	1614	8.316	-4.920	4.652	1.00	21.81
ATOM	1223	CB	LEU	1614	9.107	-3.906	5.484	1.00	19.94
ATOM	1224	CG	LEU	1614	8.609	-3.616	6.902	1.00	21.94
ATOM	1225	CD1	LEU	1614	9.580	-2.719	7.654	1.00	14.28
ATOM	1226	CD2	LEU	1614	7.227	-2.977	6.814	1.00	17.45
ATOM	1227	C	LEU	1614	8.764	-4.858	3.182	1.00	23.74
ATOM	1228	0	LEU	1614	8.169	-4.150	2.367	1.00	25.26
ATOM	1229	N	ALA	1615	9.831	-5.587	2.862	1.00	25.00
ATOM	1231	CA	ALA	1615	10.357	-5.644	1.502	1.00	23.04
ATOM	1232	CB	ALA	1615	11.710	-6.360	1.483	1.00	20.02
ATOM	1233	C	ALA	1615	9.351	-6.357	0.605	1.00	23.15
ATOM	1234	o	ALA	1615	9.076	-5.891	-0.503	1.00	25.25
ATOM	1235	N	SER	1616	8.754	-7.441	1.104	1.00	23.64
ATOM	1237	CA	SER	1616	7.758	-8.199	0.337	1.00	23.60
ATOM	1238	CB	SER	1616	7.346	-9.453	1.107	1.00	22.46
ATOM	1239	OG	SER	1616	6.531	-9.131	2.224	1.00	26.66
ATOM	1241	C	SER	1616	6.505	-7.369	0.025	1.00	25.45
ATOM	1242	0	SER	1616	5.813	-7.607	-0.967	1.00	
ATOM	1243	N	LYS	1617	6.193	-6.436	0.916	1.00	26.67
ATOM	1245	CA				-5.551			25.47
ATOM		CB	LYS	1617	5.051		0.781	1.00	25.04
	1246		LYS	1617	4.513	-5.183	2.163	1.00	26.30
ATOM	1247	CC	LYS	1617	3.778	-6.318 -6.530	2.851	1.00	28.58
ATOM	1248	CD	LYS	1617	2.438	-6.530	2.169	1.00	33.00
ATOM	1249	CE	LYS	1617	1.652	-7.676	2.764	1.00	38.57
MOTA	1250	NZ	LYS	1617	2.167	-8.987	2.300	1.00	45.15
ATOM	1254	C	LYS	1617	5.417	-4.293	0.002	1.00	26.34



ATOM	1326	CA	LEU	1624	16.905	1.469	9.216	1.00	25.91
MOTA	1327	CB	LEU:	1624	17.025	0.209	8.367	1.00	23.35
ATOM	1328	CG	LEU	1624	17.089	-1.107	9.127	1.00	21.09
ATOM	1329	CD1	LEU	1624	15.824	-1.303	10.009	1.00	14.44
ATOM	1330	CD2	LEU	1624	17.282	-2.215	8.101	1.00	18.30
ATOM	1331	С	LEU	1624	18.136	1.640	10.105	1.00	24.93
ATOM	1332	0	LEU	1624	19.235	1.897	9.611	1.00	25.58
MOTA	1333	N	ALA	1625	17.912	1.557	11.416	1.00	26.30
ATOM	1335	CA	ALA	1625	18.945	1.702	12.445	1.00	23.59
ATOM	1336	CB	ALA	1625	19.271	3.174	12.654	1.00	15.82
ATOM	1337	С	ALA	1625	18.351	1.116	13.732	1.00	23.64
ATOM	1338	0	ALA	1625	17.135	0.928	13.825	1.00	26.66
ATOM	1339	N	ALA	1626	19.197	0.815	14.712	1.00	21.59
MOTA	1341	CA	ALA	1626	18.708	0.266	15.974	1.00	21.66
ATOM	1342	CB	ALA	1626	19.860	-0.179	16.838	1.00	22.97
ATOM	1343	C	ALA	1626	17.835	1.272	16.731	1.00	24.98
MOTA	1.344	0	ALA	1626	17.072	0.891	17.620	1.00	26.84
ATOM	1345	N	ARG	1627	17.978	2.558	16.409	1.00	24.55
MOTA	1347	CA	ARG	1627	17.178	3.598	17.042	1.00	25.29
MOTA	1348	CB	ARG	1627	17.699	4.983	16.673	1.00	26.66
ATOM	1349	CG	ARG	1627	17.675	5.276	15.179	1.00	30.56
ATOM	1350	CD	ARG	1627	18.033	6.715	14.902	1.00	34.97
ATOM	1351	NE	ARG	1627	18.177	6.980	13.470	1.00	40.03
ATOM	1353	CZ	ARG	1627	19.322	6.864	12.809	1.00	40.62
ATOM	1354	NH1	ARG	1627	20.421	ნ.485	13.441	1.00	46.52
MOTA	1357	NH2	ARG	1627	19.377	7.159	11.523	1.00	43.25
ATOM	1360	C	ARG	1627	15.739				



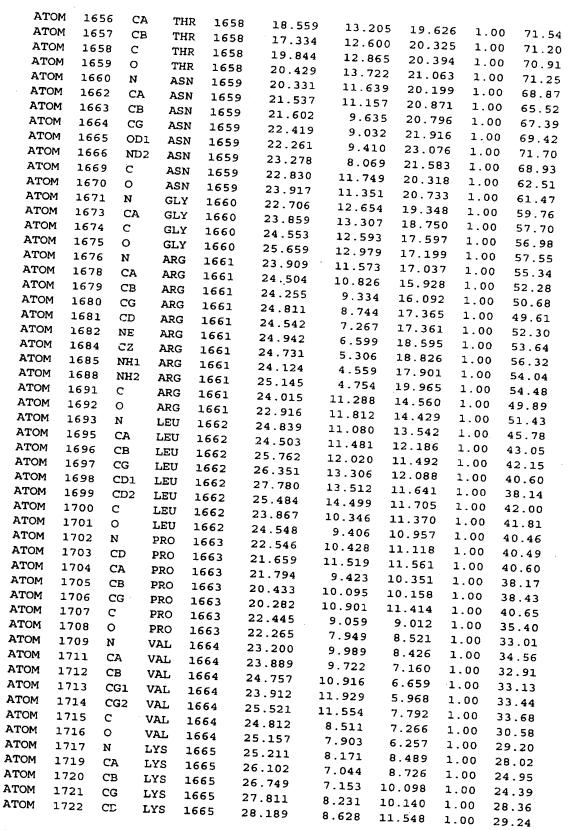
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ATOM	1459	CD	LYS	1638	6.386	-5.018	18.109	1.00	31.48
MOTA	1460	CE	LYS	1638	5.485	-6.263	18.202	1.00	27.09
MOTA	1461	NZ	LYS	1638	4.888	-6.561	16.869	1.00	26.68
MOTA	1465	C	LYS	1638	10.196	-3.208	15.416	1.00	26.56
ATOM	1466	0	LYS	1638	10.514	-2.194	16.040	1.00	27.40
ATOM	1467	N	ILE	1639	10.211	-3.271	14.092	1.00	24.31
ATOM	1469	CA	ILE	1639	10.649	-2.147	13.289	1.00	24.84
MOTA	1470	CB	ILE	1639	10.924	-2.588	11.836	1.00	25.81
ATOM	1471	CG2	ILE	1639	11.248	-1.395	10.952	1.00	24.18
ATOM	1472	CG1	ILE	1639	12.094	-3.566	11.826	1.00	25.01
ATOM	1473	CD1	ILE	1639	12.075	-4.499	10.675	1.00	27.90
ATOM	1474	C	ILE	1639	9.641	-0.999	13.348	1.00	24.90
ATOM	1475	0	ILE	1639	8.435	-1.186	13.170	1.00	25.24
ATOM	1476	N	ALA	1640	10.167	0.183	13.635	1.00	25.70
ATOM	1478	CA	ALA	1640	9.378	1.392	13.744	1.00	27.61
ATOM	1479	CB	ALA	1640	9.699	2.094	15.070	1.00	26.37
ATOM	1480	С	ALA	1640	9.637	2.348	12.576	1.00	28.35
ATOM	1481	0	ALA	1640	10.650	2.243	11.871	1.00	28.40
ATOM	1482	N	ASP	1641	8.676	3.237	12.354	1.00	29.74
ATOM	1484	CA	ASP	1641	8.760	4.272	11.325	1.00	32.13
ATOM	1485	CB	ASP	1641	9.873	5.273	11.688	1.00	34.31
ATOM	1486	CG	ASP	1641	9.507	6.158	12.896	1.00	36.31
ATOM	1487	OD1	ASP	1641	10.299	7.056	13.258	1.00	42.18
ATOM	1488	OD2	ASP	1641	8.420	5.974	13.483	1.00	41.03
MOTA	1489	C	ASP	1641	8.882	3.840	9.867	1.00	32.00
MOTA	1490	0	ASP	1641	9.339	4.617	9.021	1.00	32.65
MOTA	1491	N	PHE	1642	8.415	2.634	9.563	1.00	30.61
ATOM	1493	CA	PHE	1642	8.473	2.119	8.200	1.00	30.06
ATOM'	1494	CB	PHE	1642	8.248	0.606	8.189	1.00	24.46
ATOM	1495	CG	PHE	1642	6.981	0.176	8.854	1.00	23.26
ATOM	1496	CD1	PHE	1642	5.799	0.075	8.125	1.00	19.66
ATOM	1497	CD2	PHE	1642	6.966	-0.134	10.209	1.00	22.88
ATOM	1498	CE1	PHE	1642	4.609	-0.331	8.734	1.00	20.97
ATOM	1499	CE2	PHE	1642	5.785	-0.540	10.830	1.00	26.61
ATOM	1500	CZ	PHE	1642	4.599	-0.639	10.083	1.00	24.82
ATOM	1501	С	PHE	1642	7.512	2.830	7.225	1.00	33.14
ATOM	1502	0	PHE	1642	7.791	2.922	6.029	1.00	36.48
ATOM	1503	N	GLY	1643	6.411	3.372	7.741	1.00	32.65
ATOM	1505	CA	GLY	1643	5.462	4.059	6.876	1.00	32.28
ATOM	1506	C	GLY	1643	5.629	5.560	6.913	1.00	32.19
ATOM	1507	0	GLY	1643	4.795	6.310	6.415	1.00	30.74
ATOM	1508	N	LEU	1644	6.739	5.997	7.486	1.00	36.80
ATOM	1510	CA	LEU	1644	7.052	7.406	7.630	1.00	41.95
ATOM	1511	CB	LEU	1644	8.332	7.551	8.439	1.00	37.41
ATOM	1512	CG	LEU	1644	8.377	8.746	9.369	1.00	38.98
ATOM	1513	CD1	LEU	1644	7.384	8.548	10.493	1.00	40.45
ATOM	1514	CD2	LEU	1644	9.775	8.904	9.929	1.00	41.94
ATOM	1515	C	LEU	1644	7.189	8.150	6.296	1.00	47.55
MOTA	1516	0	LEU	1644	7.787	7.648	5.341	1.00	50.55
MOTA	1517	N	ALA	1645	6.637	9.356	6.247	1.00	52.59
MOTA	1519	CA	ALA	1645	6.686	10.194	5.055	1.00	56.88
ATOM	1520	CB	ALA	1645	5.391	10.999		1.00	58.01
ATOM	1521	С	ALA	1645	7.880	11.135	5.178	1.00	58.95



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ATOM 1587 OD1 ASP 1652 19.786 7.636 1.00 82.38 21.247 MOTA 1588 OD2 ASP 19.780 1.00 81.51 1652 20.081 9.497 MOTA 1589 С ASP 1652 20.637 16.984 6.783 1.00 72.31 **ATOM** 1590 0 ASP 1652 20.599 16.403 7.866 1.00 71.41 **ATOM** 1591 N TYR 1653 21.610 16.805 5.894 1.00 71.44 MOTA 1593 CA TYR 1653 22.736 15.900 6.143 1.00 70.07 MOTA 1594 TYR CB 1653 23.655 15.849 4.921 1.00 66.96 **ATOM** 1595 TYR CG 1653 23.153 14.932 3.834 1.00 66.43 ATOM 1596 CD1 TYR 1653 23.881 14.757 2.657 1.00 66.60 MOTA 1597 CE1 TYR 1653 23.434 13.898 1.653 1.00 68.33 ATOM 1598 CD2 TYR 1653 21.960 14.224 3.981 1.00 66.58 ATOM 1599 CE2 TYR 1653 21.500 13.363 2.990 1.00 68.84 MOTA 1600 CZTYR 1653 22.241 13.205 1.823 1.00 69.34 **ATOM** 1601 OH TYR 1653 21.781 12.360 0.833 1.00 69.88 MOTA 1603 С TYR 1653 23.557 16.227 7.391 1.00 70.80 MOTA 1604 0 TYR 1653 24.197 15.351 7.975 1.00 70.62 **ATOM** 1605 TYR 1654 23.531 N 17.488 7.802 1.00 70.76 MOTA 1607 CA TYR 1654 24.280 17.902 8.972 1.00 70.97 ATOM 1608 CB TYR 1654 24.795 19.328 8.783 1.00 69.27 MOTA 1609 CĠ TYR 1654 25.935 19.401 7.787 1.00 69.68 MOTA 1610 CD1 TYR 1654 25.696 19.352 6.415 1.00 69.51 ATOM 1611 CE1 TYR 1654 26.750 19.380 5.498 1.00 70.15 **ATOM** 1612 CD2 TYR 1654 27.256 19.482 8.221 1.00 69.92 MOTA 1613 CE2 TYR 1654 19.513 28.314 7.316 1.00 70.26 ATOM 1614 CZTYR 1654 28.057 19.462 5.958 1.00 70.22 **ATOM** 1615 OH TYR 1654 29.111 19.492 5.069 1.00 69.67 ATOM 1617 TYR 17.763 С 1654 23.503 10.272 1.00 72.19 MOTA 1618 TYR 0 1654 24.035 18.043 11.344 1.00 73.21 MOTA 1619 N LYS 1655 22.269 17.275 10.183 1.00 73.05 **ATOM** 1621 CA LYS 1655 21.424 17.108 11.363 1.00 74.81 MOTA 1622 CB LYS 1655 19.955 17.124 10.953 1.00 75.63 **MOTA** 1623 CG LYS 18.978 1655 17.239 12.102 1.00 79.16 **ATOM** 1624 CD LYS 1655 17.581 17.513 11.576 1.00 84.09 MOTA 1625 CE LYS 1655 16.517 17.244 12.634 1.00 87.56 MOTA 1626 NZ LYS 1655 15.139 17.478 12.097 1.00 89.36 ATOM 1630 C LYS 1655 21.738 15.834 1.00 12.156 75.72 MOTA 1631 0 LYS 1655 21.900 14.751 11.586 1.00 77.14 **ATOM** 1632 N LYS 1656 21.815 15.977 13.477 1.00 75.08 MOTA 1634 CA LYS 1656 22.106 14.857 14.363 1.00 73.36 MOTA 1635 CB LYS 1656 23.062 15.296 1.00 15.477 72.88 ATOM 1636 CG LYS 1656 24.475 15.599 15.007 1.00 72.87 MOTA 1637 CD LYS 1656 25.346 16.048 16.167 1.00 74.66 **ATOM** 1638 CE LYS 1656 26.830 15.945 15.828 1.00 74.84 **ATOM** 1639 NZ LYS 1656 27.701 16.322 16.981 1.00 73.74 **ATOM** 1643 С LYS 1656 20.827 14.311 14.982 1.00 72.45 ATOM 1644 0 LYS 1656 19.795 14.991 15.007 1.00 72.74 MOTA 1645 1657 20.900 1.00 N THR 13.075 15.469 71.26 MOTA 1647 THR CA 1657 19.763 12.426 16.107 1.00 70.05 ATOM 1648 CB THR 1657 19.969 10.886 16.206 1.00 68.30 ATOM 1649 OG1 THR 1657 21.084 10.598 17.060 1.00 69.34 MOTA 1651 CG<sub>2</sub> THR 1657 20.244 10.292 14.B39 1.00 66.16 ATOM 1652 C THR 1657 19.707 13.019 17.504 1.00 70.37 ATOM 1653 0 THR 1657 20.608 13.761 17.892 1.00 71.47 MOTA 1654 N THR 1658 18.669 12.691 18.263 1.00 70.80



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229 MOTA 9.690 11.489 1723 CE LYS 1665 29.269 1.00 31.15 29.639 MOTA NZ 10.194 12.836 1.00 1724 LYS 1665 35.47 MOTA 1728 C LYS 1665 25.440 5.692 8.543 1.00 25.16 MOTA 1729 О LYS 1665 26.096 4.671 8.627 1.00 24.34 MOTA 1730 N TRP 1666 24.138 5.698 8.286 1.00 25.16 ATOM 1732 CA TRP 1666 23.414 4.461 8.053 1.00 26.61 ATOM 1733 CB TRP 1666 22.157 4.412 8.917 1.00 28.17 MOTA 1734 CG TRP 1666 22.428 3.931 10.330 1.00 30.26 MOTA 1735 CD2 TRP 1666 22.930 4.714 11.426 1.00 26.92 ATOM 1736 TRP CE<sub>2</sub> 1666 23.063 3.837 12.537 1.00 26.34 MOTA 1737 CE3 TRP 1666 23.286 6.057 11.598 1.00 24.69 **ATOM** 1738 CD1 TRP 1666 22.276 2.656 10.800 1.00 26.44 MOTA 1739 NE1 TRP 1666 22.659 2.592 12.118 1.00 25.65 **ATOM** 1741 CZ2 TRP 1666 23.535 4.264 13.779 1.00 24.97 ATOM 1742 CZ3 TRP 1666 23.758 6.484 12.837 1.00 22.23 MOTA 1743 CH2 TRP 1666 23.877 5.587 13.908 1.00 24.97 MOTA 1744 C TRP 1666 23.048 4.345 6.572 1.00 27.24 1745 **ATOM** O TRP 1666 22.573 3.301 6.116 1.00 29.16 ATOM 1746 N MET 1667 23.355 5.390 5.811 1.00 26.70 ATOM 1748 CA MET 1667 23.022 5.444 4.398 1.00 25.21 MOTA 1749 CB MET 1667 22.828 6.893 3.963 1.00 28.81 MOTA 1750 CG MET 1667 21.704 7.630 4.637 1.00 35.42 MOTA 1751 SD MET 1667 21.567 9.283 3.924 1.00 42.64 ATOM 1752 CE MET 1667 20.959 8.858 2.369 1.00 41.32 MOTA 1753  $\mathbf{C}$ MET 1667 23.984 4.807 3.417 1.00 25.03 MOTA 1754 0 MET 1667 25.182 5.047 3.446 1.00 24.24 2.501 MOTA 1755 N ALA 1668 23.420 4.034 1.00 26.70 MOTA 1757 CA ALA 1668 24.186 3.398 1.441 1.00 27.82 MOTA 1758 CB ALA 1668 2.509 23.272 0.601 1.00 25.36 ATOM 1759 С ALA 1668 4.528 0.575 1.00 24.738 28.42 ATOM 1760 0 ALA 1668 24.044 5.521 0.321 1.00 27.52 MOTA 1761 N PRO 1669 25.972 0.065 28.95 4.374 1.00 ATOM 1762 PRO 1669 CD 26.867 3.214 0.170 1.00 27.98 MOTA 1763 CA PRO 1669 26.571 5.418 -0.775 1.00 28.76 MOTA 1764 CB PRO 1669 27.814 4.731 -1.326 1.00 28.58 MOTA 1765 CG PRO 1669 28.193 3.809 -0.209 1.00 30.22 **ATOM** 1766 PRO 1669 C 25.647 5.909 -1.893 1.00 27.08 **ATOM** 1767 0 PRO 1669 25.496 7.107 -2.093 1.00 28.31 ATOM 1768 N GLU 1670 24.993 4.997 -2.595 1.00 25.42 **ATOM** 1770 CA GLU 1670 24.110 5.423 -3.673 1.00 27.02 **ATOM** 1771 CB GLU 1670 23.680 4.233 -4.542 1.00 27.18 **ATOM** 1772 CG GLU 1670 22.662 3.294 -3.911 1.00 27.66 **ATOM** 1773 CD GLU 1670 23.280 2.162 -3.112 1.00 27.75 MOTA OE1 1774 GLU 1670 22.488 1.309 -2.647 1.00 27.12 MOTA 1775 OE2 GLU 1670 24.526 2.114 -2.944 1.00 21.64 **ATOM** 1776 С GLU 1670 22.896 6.229 -3.189 1.00 26.88 ATOM 1777 0 GLU 1670 22.348 7.037 -3.929 1.00 24.52 MOTA -1.948 1778 N ALA 1671 22.477 6.009 1.00 29.43 MOTA 1780 ALA CA 1671 21.342 6.744 -1.392 1.00 29.29 MOTA 1781 CB ALA 1671 20.751 5.989 -0.217 1.00 26.98 MOTA 1782 C ALA 1671 21.826 **B.124** -0.939 1.00 31.14 ATOM 1783 0 ALA 1671 21.159 9.135 -1.143 1.00 31.67 MOTA 1784 N LEU 1672 23.013 8.139 -0.343 1.00 32.31

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CA

LEU

1672

23.636

9.352

0.154

1.00

33.79

MOTA



7,000		_							
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ATO	_		1 LEC	J 1672	24.713	10.840			
ATO			2 LEC	J 1672	26.863	9.665			
ATO		_	LEU	1672	24.078	10.280			55
ATO		2 0	LEU	1672	23.789	11.478			
ATO	•	3 N	PHE	1673	24.770	9.723			-
ATO			PHE	1673	25.266	10.504			
ATO		CB	PHE	1673	26.553	9.874			
ATO		7 CG	PHE	1673	27.661	9.761			
MOTA		CD1	PHE	1673	28.313	8.545			
ATON		CD2	PHE	1673	28.055	10.867			
ATON		CE1	PHE	1673	29.346	8.419	-1.861		34.87
ATOM		CE2	PHE	1673	29.090	10.757	-1.484	1.00	31.98
ATOM		CZ	PHE	1673	29.736		-0.919	1.00	36.31
ATOM		C	PHE	1673	24.273	9.525 10.670	-0.732	1.00	34.55
ATOM		_	PHE	1673	24.135		-4.217	1.00	34.79
ATOM	1805	N	ASP	1674	23.584	11.754	-4.765	1.00	35.74
ATOM	1807	CA	ASP	1674	22.650	9.588	-4.572	1.00	37.31
ATOM	1808	CB	ASP	1674	22.917	9.601	-5.698	1.00	35.61
ATOM	1809	CG	ASP	1674	24.362	8.392	-6.600	1.00	37.01
ATOM	1810	OD1	ASP	1674	25.030	8.288	-7.041	1.00	41.02
ATOM	1811	OD2	ASP	1674	24.828	9.340	-7.194	1.00	43.07
MOTA	1812	C	ASP	1674	21.162	7.145	-7.251	1.00	42.24
MOTA	1813	0	ASP	1674	20.315	9.632	-5.360	1.00	37.06
ATOM	1814	N	ARG	1675	20.315	9.506	-6.257	1.00	36.37
ATOM	1816	CA	ARG	1675	19.445	9.745	-4.077	1.00	37.78
ATOM	1817	CB	ARG	1675	18.832	9.791	-3.650	1.00	39.41
ATOM	1818	CG	ARG	1675		11.137	-4.039	1.00	44.39
MOTA	1819	CD	ARG	1675	19.413	12.299	-3.269	1.00	54.30
ATOM	1820	NE	ARG	1675	19.516	13.551	-4.127	1.00	63.84
ATOM	1822	CZ	ARG	1675	20.060	14.664	-3.349	1.00	73.69
ATOM	1823	NH1	ARG	1675	19.652	15.925	-3.453	1.00	77.10
ATOM	1826	NH2	ARG	1675	18.695	16.253	-4.312	1.00	79.65
ATOM	1829	C	ARG	1675	20.177	16.855	-2.665	1.00	79.31
ATOM	1830	ō	ARG		18.617	8.639	-4.221	1.00	37.46
ATOM	1831	N	ILE	1675 1676	17.447	8.808	4.557	1.00	38.57
ATOM	1833	CA	ILE		19.235	7.475	-4.351	1.00	34.37
ATOM	1834	CB	ILE	1676	18,545	6.313	-4.874	1.00	32.99
ATOM	1835	CG2	ILE	1676	19.358	5.644	-5.976	1.00	33.98
ATOM	1836	CG1	ILE	1676	18.552	4.529	-6.602	1.00	35.04
ATOM	1837	CD1	ILE	1676	19.708	6.663	-7.050	1.00	34.92
ATOM	1838	C		1676	20.799	6.200	-7.962	1.00	41.16
ATOM	1839	0	ILE	1676	18.315	5.315	-3.743	1.00	31.55
ATOM	1840	N	ILE	1676	19.245	4.632	-3.300	1.00	30.65
ATOM	1842	CA	TYR	1677	17.082	5.279	-3.246	1.00	30.88
ATOM	1843	CB	TYR	1677	16.701	4.371	-2.173	1.00	27.10
ATOM	1844		TYR	1677	15.771	5.074	-1.208		28.30
ATOM	1845	CG	TYR	1677	16.457	6.136	-0.406		30.61
ATOM		CD1		1677	16.598	7.432			30.82
ATOM	1846	CE1		1677	17.212	8.424			30.75
ATOM	1847	CD2		1677	16.952	5.857			29.75
ATOM	1848	CE2		1677	17.567	6.842			32.62
	1849	CZ		1677	17.688	8.125			34.51
ATOM	1850	OH	TYR	1677	18.238	9.118	_		
								00	38.89

ATOM	1852	С	TYR	1677	16.029	3.149	-2.743	1.00	25.47
ATOM	1853	0	TYR	1677	15.132	3.264	-3.578	1.00	26.00
MOTA	1854	N	THR	1678	16.459	1.983	-2.272	1.00	24.27
ATOM	1856	CA	THR	1678	15.942	0.701	-2.734	1.00	24.09
MOTA	1857	CB	THR	1678	16.830	0.123	-3.853	1.00	24.19
ATOM	1858	OG1	THR	1678	18.165	-0.008	-3.349	1.00	27.81
MOTA	1860	CG2	THR	1678	16.843	1.009	-5.085	1.00	24.15
ATOM	1861	C	THR	1678	15.979	-0.297	-1.577	1.00	25.02
ATOM	1862	0	THR	1678	16.379	0.036	-0.465	1.00	27.65
MOTA	1863	N	HIS	1679	15.569	-1.530	-1.844	1.00	25.04
MOTA	1865	CA	HIS	1679	15.591	-2.560	-0.818	1.00	24.35
MOTA	1866	CB	HIS	1679	14.853	-3.812	-1.298	1.00	23.78
MOTA	1867	CG	HIS	1679	13.390	-3.592	-1.536	1.00	27.24
MOTA	1868	CD2	HIS	1679	12.627	-3.758	-2.643	1.00	28.22
ATOM	1869	ND1	HIS	1679	12.532	-3.137	-0.551	1.00	30.64
ATOM	1871	CE1	HIS	1679	11.310	-3.028	-1.041	1.00	28.13
ATOM	1872	NE2	HIS	1679	11.339	-3.400	-2.307	1.00	28.52
ATOM	1874	C	HIS	1679	17.056	-2.846	-0.514	1.00	22.52
MOTA	1875	0	HIS	1679	17.419	-3.179	0.613	1.00	22.58
ATOM	1876	N	GLN	1680	17.898	-2.604	-1.516	1.00	24.34
ATOM	1878	CA	GLN	1680	19.341	-2.800	-1.406	1.00	23.52
MOTA	1879	CB	GLN	1680	19.998	-2.781	-2.782	1.00	25.36
ATOM	1880	CG	GLN	1680	19.741	-4.050	-3 577	1.00	33.28
ATOM	1881	CD	GLN	1680	19.212	-3.763	-4.949	1.00	34.68
ATOM	1882	OE1	GLN	1680	18.683	-2.686	-5.187	1.00	41.24
ATOM	1883	NE2	GLN	1680	19.357	-4.713	-5.867	1.00	32.10
ATOM	1886	C	GLN	1680	19.998	-1.767	-0.514	1.00	23.38
ATOM	1887	0	GLN	1680	20.925	-2.094	0.224	1.00	25.12
ATOM	1888	N	SER	1681	19.533	-0.521	-0.562	1.00	20.87
MOTA	1890	CA	SER	1681	20.133	0.480	0.303	1.00	20.53
ATOM	1891	CB	SER	1681	19.821	1.919	-0.151	1.00	19.58
MOTA	1892	OG	SER	1681	18.445	2.126	-0.425	1.00	20.67
ATOM	1894	C	SER	1681	19.696	0.189	1.741	1.00	22.22
ATOM	1895	0	SER	1681	20.439	0.455	2.681	1.00	23.62
ATOM	1896	N	ASP	1682	18.530	-0.436	1.900	1.00	22.44
ATOM	1898	CA	ASP	1682	18.054	-0.816	3.231	1.00	22.70
ATOM	1899	CB	ASP	1682	16.607	-1.293	3.180	1.00	24.24
ATOM	1900	CG	ASP	1682	15.603	-0.165	3.352	1.00	28.23
ATOM	1901	OD1	ASP	1682	14.410	-0.425	3.108	1.00	28.14
ATOM	1902	OD2	ASP	1682	15.976	0.960	3.757	1.00	25.23
ATOM	1903	C	ASP	1682	18.926	-1.941	3.777	1.00	23.92
ATOM	1904	0	ASP	1682	19.121	-2.057	4.990	1.00	26.24
ATOM	1905	N	VAL	1683	19.433	-2.788	2.884	1.00	23.67
ATOM	1907	CA	VAL	1683	20.300	-3.888	3.302	1.00	22.42
ATOM	1908	CB	VAL	1683	20.562	-4.881	2.141	1.00	23.70
ATOM	1909	CG1	VAL	1683	21.724	-5.802	2.459	1.00	19.73
ATOM	1910	CG2	VAL	1683	19.292	-5.713	1.889	1.00	19.85
MOTA	1911	С	VAL	1683	21.584	-3.298	3.860	1.00	21.94
MOTA	1912	0	VAL	1683	22.030	-3.688	4.938	1.00	22.69
ATOM	1913	N	TRP	1684	22.141	-2.320	3.154	1.00	20.51
ATOM	1915	CA	TRP	1684	23.349	-1.633	3.611	1.00	20.31
ATOM	1916	CB	TRP	1684	23.659	-0.446	2.680	1.00	19.01
ATOM	1917	CG	TRP	1684	24.802	0.410	3.145	1.00	20.67
ATOM	1918	CD2	TRP	1684	26.114	0.468	2.587	1.00	22.26



ATO	M 191	9 CE:	2 TRI	7604	26.000				
ATO					•			3 1.00	21.22
ATO					26.718			3 1.00	22.51
ATO					24.825	1.229		1.00	19.91
ATO					26.079			1.00	18.59
ATO					28.236	1.586			
ATO					28.059	0.141	1.204		
ATO						0.992	2.047		23.34
ATO		_	TRP	•	23.131	-1.150	5.069		21.49
ATO		_	TRP		23.958	-1.412	5.954		23.34
ATOM			SER		22.015	-0.463	5.308		21.84
	_		SER		21.652	0.042			20.02
4OTA			SER	1685	20.310	0.773			19.12
ATOM	_		SER	1685	20.335	1.791		1.00	21.62
ATOM			SER	1685	21.551	-1.111		1.00	22.64
ATOM		-	SER	1685	21.908	-0.946	8.829	1.00	
ATOM			PHE	1686	21.043	-2.266	7.202	1.00	22.09
ATOM			PHE	1686	20.939	-3.438	8.075	1.00	22.44
ATOM			PHE	1686	20.196	-4.588	7.380	1.00	22.91
ATOM		CG	PHE	1686	20.027	-5.808	8.256		23.75
ATOM		CD1	PHE	1686	19.220	-5.757	9.388	1.00	23.61
ATOM		CD2	PHE	1686	20.731	-6.976	7.990	1.00	21.21
ATOM		CE1	PHE	1686	19.118	-6.836	10.240	1.00	23.91
ATOM		CE2	PHE	1686	20.636	-8.074	8.841	1.00	20.66
ATOM	1946	CZ	PHE	1686	19.828	-7.999	9.972	1.00	22.47
ATOM	1947	C	PHE	1686	22.339	-3.904		1.00	23.35
ATOM	1948	o	PHE	1686	22.526	-4.382	8.522	1 00	22.60
ATOM	1949	N	GLY	1687	23.312	-3.770	9.646	1.00	22.83
ATOM	1951	CA	GLY	1687	24.682	-4.140	7.626	1.00	23.82
ATOM	1952	C	GLY	1687	25.175		7.941	1.00	22.58
ATOM	1953	0	GLY	1687	25.832	-3.262 -3.749	9.071	1.00	21.49
ATOM	1954	N	VAL	1688	24.849		9.990	1.00	21.62
ATOM	1956	CA	VAL	1688	25.229	.1.968	9.008	1.00	21.15
ATOM	1957	CB	VAL	1688	24.894	-1.008	10.052	1.00	20.56
MOTA	1958	CG1	VAL	1688	25.408	0.479	9.647	1.00	17.69
ATOM	1 <b>9</b> 59	CG2	VAL	1688	25.518	1.456	10.690	1.00	15.11
ATOM	1960	C	VAL	1688	24.494	0.821	8.314	1.00	11.54
ATOM	1961	0	VAL	1688		-1.398	11.346	1.00	22.60
ATOM	1962	N	LEU	1689	25.083 23.215	-1.407	12.428	1.00	25.23
ATOM	1964	CA	LEU	1689		-1.755	11.229	1.00	26.09
ATOM	1965	CB	LEU	1689	22.423	-2.175	12.387	1.00	25.16
ATOM	1966	CG	LEU	1689	20.976	-2.455	11.965	1.00	25.91
MOTA	1967	CD1	LEU	1689	19.913	-2.560	13.068	1.00	27.54
ATOM	1968	CD2	LEU	1689	18.557	-2.241	12.496	1.00	28.11
MOTA	1969	C	LEU		19.898	-3.940	13.704	1.00	31.67
ATOM	1970	0	LEU	1689	23.055	-3.426	13.018	1.00	27.49
ATOM	1971	N		1689	23.128	-3.532	14.246		28.99
ATOM	1973	CA	LEU	1690	23.485	-4.374	12.180	1.00	27.67
ATOM	1974		LEU	1690	24.149	-5.596	12.643		26.76
ATOM		CB	LEU	1690	24.616	-6.453	11.456		28.58
ATOM	1975	CG	LEU	1690	23.651	-7.406	10.733		29.46
ATOM	1976	CD1		1690	24.372	-8.064	9.565		27.79
ATOM	1977	CD2		1690	23.130	-8.488	11.691		28.15
	1978	C		1690	25.362	-5.176			26.19
MOTA	1979	0		1690	25.565	-5.670			25.29
ATOM	1980	N	TRP	1691	26.124	-4.217			25.29 25.89
									0 7

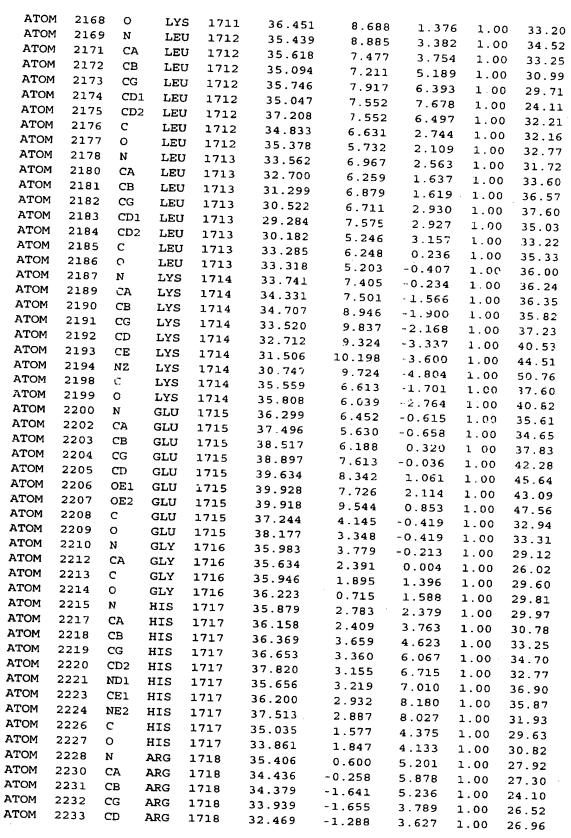


MOTA	1982	CA	TRP	1691	27.302	-3.682	13.631	1.00	27.31
ATOM	1983	CB	TRP	1691	27.979	-2.628	12.755	1.00	25.21
MOTA	1984	CG	TRP	1691	29.338	-2.170	13.257	1.00	27.00
MOTA	1985	CD2	TRP	1691	29.606	-1.060	14.134	1.00	24.28
ATOM	1986	CE2	TRP	1691	31.001	-0.988	14.297	1.00	23.03
MOTA	1987	CE3	TRP	1691	28.792	-0.118	14.778	1.00	22.80
ATOM	1988	CD1	TRP	1691	30.562	-2.712	12.944	1.00	24.10
ATOM	1989	NE1	TRP	1691	31.557	-2.010	13.567	1.00	23.41
MOTA	1991	CZ2	TRP	1691	31.617	-0.011	15.097	1.00	25.00
ATOM	1 <b>9</b> 92	CZ3	TRP	1691	29.398	0.851	15.573	1.00	26.78
ATOM	1993	CH2	TRP	1691	30.802	0.900	15.719	1.00	27.78
MOTA	1994	C	TRP	1691	26.947	-3.088	15.012	1.00	28.70
ATOM	1995	O	TRP	1691	27.708	-3.245	15.974	1.00	29.56
MOTA	1996	N	GLU	1692	25.808	-2.400	15.104	1.00	29.51
MOTA	1998	CA	GLU	1692	25.349	-1.817	16.371	1.00	27.55
ATOM	1999	CB	GLU	1692	24.120	-0.935	16.171	1.00	28.35
ATOM	2000	CG	GLU	1692	24.273	0.221	15.219	1.00	24.70
ATOM	2001	CD	GLU	1692	22.982	0.989	15.100	1.00	25.44
ATOM	2002	OE1	GLU	1692	22.224	0.744	14.148	1.00	24.34
ATOM	2003	OE2	GLU	1692	22.696	1.816	15.982	1.00	27.57
ATOM	2004	С	GLU	1692	24.958	-2.918	17.352	1.00	28.74
MOTA	2005	0	GLU	1692	25.099	-2.753	18.557	1.00	28.76
ATOM	2006	N	ILE	1693	24.421	-4.023	16.844	1.00	29.23
ATOM	2008	CA	ILE	1693	24.027	-5.125	17.712	1.00	27.48
ATOM	2009	CB	ILE	1693	23.205	-6.226	16.944	1.00	28.80
ATOM	2010	CG2	ILE	1693	22.983	-7.469	17.842	1.00	22.98
ATOM	2011	CG1	ILE	1693	21.840	-5.658	16.508	1.00	27.36
ATOM	2012	CD1	ILE	1693	21.005	6.585	15.635	1.00	24.84
ATOM	2013	С	ILE	1693	25.259	-5.750	18.357	1.00	27.27
ATOM	2014	0	ILE	1693	25.320	-5.902	19.575	1.00	28.15
ATOM	2015	N	PHE	1694	26.273	-6.043	17.552	1.00	27.83
ATOM	2017	CA	PHE	1694	27.473	-6.677	18.095	1.00	29.88
ATOM	2018	CB	PHE	1694	28.143	-7.525	17.011	1.00	28.66
MOTA	2019	CG	PHE	1694	27.223	-8.574	16.463	1.00	29.92
MOTA	2020	CD1	PHE	1694	26.628	-8.424	15.220	1.00	30.20
MOTA	2021	CD2	PHE	1694	26.809	-9.630	17.269	1.00	30.81
MOTA	2022	CE1	PHE	1694	25.625	-9.294	14.801	1.00	32.42
MOTA	2023	CE2	PHE	1694	25.805	-10.508	16.857	1.00	32.30
MOTA	2024	CZ	PHE	1694	25.210	-10.337	15.628	1.00	31.13
ATOM	2025	C	PHE	1694	28.429	-5.784	18.890	1.00	31.07
MOTA	2026	0	PHE	1694	29.376	-6.273	19.509	1.00	33.16
MOTA	2027	N	THR	1695	28.157	-4.480	18.897	1.00	29.20
ATOM	2029	CA	THR	1695	28.934	-3.532	19.670	1.00	27.38
ATOM	2030	CB	THR	1695	29.412	-2.333	18.823	1.00	24.77
MOTA	2031	OG1	THR	1695	28.287	-1.652	18.274	1.00	26.27
ATOM	2033	CG2	THR	1695	30.305	-2.800	17.706	1.00	20.18
ATOM	2034	С	THR	1695	28.053	-3.034	20.822	1.00	29.84
MOTA	2035	0	THR	1695	28.430	-2.103	21.548	1.00	32.77
ATOM	2036	N	LEU	1696	26.898	-3.687	20.988	1.00	28.52
ATOM	2038	CA	LEU	1696	25.915	-3.364	22.029	1.00	28.82
ATOM	2039	СВ	LEU	1696	26.356	-3.886	23.394	1.00	32.50
ATOM	2040	CG	LEU	1696	26.658	-5.379	23.476	1.00	33.24
ATOM	2041	CD1	LEU	1696	27.205	-5.717	24.849	1.00	34.15
ATOM	2042	CD2	LEU	1696	25.398	-6.150	23.191	1.00	37.24



ATO	M 204	13 C	LE	U 1696	25.553	_ 1 00	0 22 12.		
ATO	M 204	4 0	LE						
ATO	M 204	5 N	GL		-0.0.5				
ATO	M 204	7 CA			24.767				·
MOTA	M 204	8 C	GL:		25.927				27.40
NOTA	1 204	9 0	GL		25.927			_	
MOTA	1 205	0 N	GL	<del>-</del> -	26.888				
ATOM	1 205	2 CA			28.031	0.416			27.26
ATOM	1 205	3 C	GLY		27.651	1.212			
ATOM	1 205	4 0	GLY		26.669	2.301			31.17
ATOM	205	5 ท	SER		28.418	2.177			33.73
ATOM	205	7 CA	SER		28.168	3.380			29.96
ATOM	2058	3 СВ	SER		28.438	4.491		-	29.37
ATOM	205		SER		28.575	5.810		1.00	31.77
ATOM	2061	C	SER		29.093	6.919		1.00	38.42
ATOM	2062	2 0	SER		30.299	4.350		1.00	27.98
ATOM	2063	N	PRO		28.537	4.310	16.529	1.00	28.18
ATOM	2064	CD	PRO	1700	27.104	4.240	15.153	1.00	29.62
ATOM	2065	CA	PRO	1700	29.381	4.259	14.794	1.00	31.22
MOTA	2066	СВ	PRO	1700	28.356	4.107	13.958	1.00	28.95
ATOM	2067	CG	PRO	1700	27.095	4.003	12.807	1.00	27.21
ATOM	2068	C	PRO	1700	30.205	3.556	13.460	1.00	29.33
ATOM	2069	0	PRO	1700	29.737	5.379	13.773	1.00	28.78
ATOM	2070	N	TYR	1701	31.426	6.469	14.110	1.00	30.04
MOTA	2072	CA	TYR	1701	32.296	5.239	13.264	1.00	28.35
ATOM	2073	CB	TYR	1701	31.921	6.390	12.987	1.00	30.77
ATOM	2074	CG	TYR	1701	32.060	6.987	11.615	1.00	31.67
MOTA	2075	CD1	TYR	1701	30.952	6.037	10.454	1.00	34.61
ATOM	2076	CE1	TYR	1701	31.083	5.673	9.686	1.00	38.26
ATOM	2077	CD2	TYR	1701	33.301	4.806	8.587	1.00	40.99
ATOM	2078	CE2	TYR	1701	33.449	5.520 4.662	10.106	1.00	38.16
ATOM	2079	CZ	TYR	1701	32.343	4.312	9.020	1.00	41.04
MOTA	2080	ОН	TYR	1701	32.531	3.478	8.263	1.00	43.11
ATOM	2082	С	TYR	1701	32.305	7.532	7.181	1.00	49.53
ATOM	2083	0	TYR	1701	32.026	8.689	14.029	1.00	31.41
MOTA	2084	N	PRO	1702	32.635	7.230	13.698	1.00	33.59
MOTA	2085	CD	PRO	1702	32.998	5.938	15.296	1.00	30.92
ATOM	2086	CA	PRO	1702	32.656	8.283	15.888	1.00	32.30
ATOM	2087	CB	PRO	1702	33.123	7.548	16.314	1.00	30.05
ATOM	2088	CG	PRO	1702	32.676	6.174	17.561 17.338	1.00	27.77
ATOM	2089	C	PRO	1702	33.659	9.366	15.944	1.00	32.34
MOTA	2090	0	PRO	1702	34.769	9.055	15.513	1.00	31.42
ATOM	2091	N	GLY	1703	33.257	10.627	16.117	1.00	30.95
ATOM	2093	CA	GLY	1703	34.122	11.751	15.817	_	31.30
ATOM	2094	C	GLY	1703	34.172	12.138		_	29.66
ATOM	2095	0	GLY	1703	34.752	13.165			31.00
ATOM	2096	N	VAL	1704	33.551	11.331			30.69
ATOM	2098	CA	VAL	1704	33.553	11.610			31.11
	2099	CB	VAL	1704	33.539	10.310			29.88
	2100	CG1	VAL	1704	33.585	10.510			28.41
	2101	CG2	VAL	1704	34.702	9.429			26.24
	2102	C		1704	32.396	12.508			24.10
	2103	0		1704	31.224				30.80
MOTA	2104	N		1705	32.718				32.50
				-		±3.705	11.104	1.00	30.86

ATOM	2105	CD	PRO	1705	34.039	14.350	11.077	1.00	30.59
ATOM	2106	CA	PRO	1705	31.682	14.625	10.645	1.00	31.47
ATOM	2107	CB	PRO	1705	32.400	15.971	10.680	1.00	32.75
MOTA	2108	CG	PRO	1705	33.774	15.607	10.289	1.00	32.59
ATOM	2109	C	PRO	1705	31.258	14.264	9.239	1.00	32.19
ATOM	2110	0	PRO	1705	31.974	13.536	8.549	1.00	33.91
MOTA	2111	N	VAL	1706	30.124	14.814	8.806	1.00	32.57
ATOM	2113	CA	VAL	1706	29.560	14.576	7.474	1.00	31.80
ATOM	2114	CB	VAL	1706	28.483	15.632	7.172	1.00	34.66
ATOM	2115	CG1	VAL	1706	28.022	15.538	5.738	1.00	39.06
MOTA	2116	CG2	VAL	1706	27.309	15.455	8.106	1.00	36.62
ATOM	2117	C	VAL	1706	30.578	14.560	6.320	1.00	31.58
MOTA	2118	0	VAL	1706	30.682	13.585	5.570	1.00	32.35
MOTA	2119	N	GLU	1707	31.326	15.649	6.189	1.00	31.46
MOTA	2121	CA	GLU	1707	32.329	15.788	5.139	1.00	31.68
ATOM	2122	CB	GLU	1707	33.021	17.148	5.267	1.00	32.59
ATOM	2123	C	GLU	1707	33.381	14.678	5.114	1.00	32.23
ATOM	2124	0	GLU	1707	33.740	14.183	4.050	1.00	33.47
ATOM	2125	N	GLU	1708	33.902	14.316	6.279	1.00	32.90
ATOM	2127	CA	GLU	1708	34.909	13.268	6.352	1.00	33.86
MOTA	2128	CB	GLU	1708	35.570	13.244	7.730	1.00	38.54
ATOM	2129	CG	GLU	1708		14.575	8.165	1.00	47.63
ATOM	2130	CD	GLU	1708	37.442	14.962	7.383	1.00	58.35
ATOM	2131	OE1	GLU	1708	38.117	14.067	6.816	1.00	62.88
MOTA	2132	OE2	GLU	1708	37.770	16.176	7.355	1.00	64.79
ATOM	2133	C	GLU	1708	34.276	11.921	6.043	1.00	33.56
ATOM	2134	0	GLU	1708	34.927	11.038	5.489	1.00	34.18
ATOM	2135	N	LEU	1709	32.997	11.774	6.374	1.00	32.91
ATOM	2137	CA	LEU	1709	32.285	10.532	6.108	L.00	33.83
ATOM ATOM	2138	CB	LEU	1709	30.862	10.563	6.685	1.00	32.28
ATOM	2139 2140	CG CD1	LEU LEU	1709	30.015	9.363	6.231	1.00	32.92
ATOM	2140	CD1	LEU	1709 1 <b>70</b> 9	30.541	8.071	6.853	1.00	28.37
ATOM	2142	CD2	LEU	1709	28.563	9.580	6.568	1.00	31.90
ATOM	2143	0	LEU	1709	32.222 32.412	10.283 9.152	4.60€ 4.15€	1.00	34.15
ATOM	2144	N	PHE	1710	31.918	11.332	4.156 3.844	1.00	34.75
ATOM	2146	CA	PHE	1710	31.828	11.332		1.00	33.83
ATOM	2147	CB	PHE	1710	31.528	12.622	2.388 1.787		32.90
ATOM	2148	CG	PHE	1710	30.162	13.132	2.082	1.00	34.85 38.60
ATOM	2149	CD1	PHE	1710	29.150	12.268	2.469	1.00	43.69
ATOM	2150	CD2	PHE	1710	29.882	14.480	1.984	1.00	45.10
ATOM	2151	CEl	PHE	1710	27.873	12.742	2.764	1.00	46.23
ATOM	2152	CE2	PHE	1710	28.611	14.966	2.274	1.00	48.15
ATOM	2153	CZ	PHE	1710	27.603	14.086	2.670	1.00	46.90
ATOM	2154	C	PHE	1710	33.131	10.739	1.803	1.00	31.84
ATOM	2155	0	PHE	1710	33.134	9.931	0.877	1.00	29.97
ATOM	2156	N	LYS	1711	34.231	11.224	2.373	1.00	32.45
ATOM	2158	CA	LYS	1711	35.582	10.860	1.947	1.00	34.53
ATOM	2159	СВ	LYS	1711	36.588	11.755	2.675	1.00	36.17
ATOM	2160	CG	LYS	1711	38.008	11.669	2.182	1.00	41.07
ATOM	2161	CD	LYS	1711	38.912	12.582	3.001	1.00	46.23
ATOM	2162	CE	LYS	1711	40.311	12.648	2.418	1.00	51.79
ATOM	2163	NZ	LYS	1711	41.036	11.360	2.556	1.00	57.27
ATOM	2167	С	LYS	1711	35.867	9.375	2.215	1.00	33.82
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MOTA	2234	NE	ARG	1718	32.020	-1.374	2.232	1.00	24.41
MOTA	2236	CZ	ARG	1718	32.090	-0.377	1.352	1.00	25.51
MOTA	2237	NH1	ARG	1718	32.611	0.801	1.706	1.00	23.61
MOTA	2240	NH2	ARG	1718	31.553	-0.521	0.149	1.00	21.28
ATOM	2243	C	ARG	1718	34.881	-0.384	7.330	1.00	28.81
MOTA	2244	0	ARG	1718	36.080	-0.425	7.611	1.00	29.77
ATOM	2245	N	MET	1719	33.920	-0.377	8.250	1.00	30.40
ATOM	2247	CA	MET	1719	34.215	-0.485	9.673	1.00	30.62
MOTA	2248	CB	MET	1719	32.942	-0.339	10.497	1.00	28.91
MOTA	2249	CG	MET	1719	32.235	1.003	10.316	1.00	30.85
ATOM	2250	SD	MET	1719	30.829	1.237	11.432	1.00	33.27
ATOM	2251	CE	MET	1719	29.521	0.416	10.561	1.00	31.81
ATOM	2252	C	MET	1719	34.900	-1.793	10.005	1.00	31.32
ATOM	2253	0	MET	1719	34.755	-2.769	9.278	1.00	31.47
ATOM	2254	N	ASP	1720	35.651	-1.799	11.103	1.00	33.78
ATOM	2256	CA	ASP	1720	36.387	-2.983	11.550	1.00	33.45
MOTA	2257	CB	ASP	1720	37.478	-2.580	12.546	1.00	36.99
ATOM	2258	CG	ASP	1720	38.585	-1.762	11.908	1.00	41.56
ATOM	2259	OD1	ASP	1720	38.403	-1.339	10.742	1.00	48.43
MOTA	2260	OD2	ASP	1720	39.634	-1.546	12.568	1.00	40.99
MOTA	2261	С	ASP	1720	35.473	-4.001	12.211	1.00	32.12
ATOM	2262	0	ASP	1720	34.381	-3.657	12.668	1.00	30.89
ATOM	2263	N	LYS	1721	35.944	-5.241	12.328	1.00	31.82
ATOM	2265	CA	LYS	1721	35.127	-6.270	12.953	1.00	31.71
ATOM	2266	CB	LYS	1721	35.691	-7.679	12.747	1.00	32.34
MOTA	2267	CG	LYS	1721	34.762	-8.738	13.344	1.00	34.85
ATOM	2268	CD	LYS	1721	35.111	-10.155	12.961	1.00	37.39
ATOM	2269	CE	LYS	1721		-10.674	13.765	1.00	41.42
ATOM	2270	ΝZ	LYS	1721	36.348	-12.154	13.635	1.00	46.55
ATOM	2274	C	LYS	1721	35.007	-6.018	14.430	1.00	33.40
ATOM	2275	0	LYS	1721	36.017	-5.879	15.121	1.00	34.26
ATOM	2276	N	PRO	1722	33.768	-5.924	14.934	1.00	34.26
ATOM	2277	CD	PRO	1722	32.494	-6.002	14.203	1.00	32.16
ATOM	2278	CA	PRO	1722	33.546	-5.692	16.362	1.00	35.84
ATOM	2279	. CB	PRO	1722	32.027	-5.682	16.473	1.00	35.35
ATOM	2280	CG	PRO	1722	31.575	-5.255	15.108	1.00	35.35
ATOM	2281	С	PRO	1722	34.105	-6.904	17.099	1.00	40.41
ATOM	2282	0	PRO	1722	34.010	-8.038	16.607	1.00	41.14
MOTA	2283	N	SER	1723	34.739	-6.680	18.240	1.00	43.60
ATOM	2285	CA	SER	1723	35.260	-7.808	18.999	1.00	45.51
ATOM	2286	CB	SER	1723	36.078	-7.324	20.191	1.00	45.30
ATOM	2287	OG	SER	1723	35.384	-6.300	20.879	1.00	49.62
MOTA	2289	C	SER	1723	34.031	-8.589	19.460	1.00	46.39
MOTA	2290	0	SER	1723	32.939	-8.028	19.614	1.00	45.16
ATOM	2291	N	ASN	1724	34.199	-9.891	19.631	1.00	48.53
MOTA	2293	CA	ASN	1724	33.088	-10.723	20.065	1.00	51.13
MOTA	2294	CB	ASN	1724	32.509	-10.194	21.390	1.00	56.87
ATOM	2295	CG	ASN	1724	33.595	-9.892	22.427	1.00	61.65
ATOM	2296	OD1	ASN	1724	34.503	-10.702	22.649	1.00	63.73
MOTA	2297	ND2	ASN	1724	33.526	-8.713	23.039	1.00	64.64
ATOM	2300	С	ASN	1724	32.034	-10.743	18.941	1.00	48.83
ATOM	2301	0	ASN	1724	30.846	-10.534	19.145	1.00	50.50
ATOM	2302	N	CYS	1725	32.511	-10.977	17.734	1.00	45.23
ATOM	2304	CA	CYS	1725	31.654	-11.056	16.570	1.00	42.33
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ATC	DM 230	)5 CI	3 CY	S 1725	31.57	0 -9.702	15 05		
ATO		)6 S(	G CY						
ATO		_	CY						
ATO		8 0	CY.						
ATO			TH	R 1726	31.664		15.579		
ATO			THI		32.275		15.263		35.96
ATO	M 231	2 CB	THI		31.301		14.459		33.61
ATO			1 THE		30.071		14.326		33.29
OTA			2 THE		30.981	~	13.711		34.53
ATO			THE		32.720		15.696		25.84
ATO		7 0	THE		32.257		13.092		32.27
ATON		8 N	ASN		33.643		12.643		33.04
AO'I'A			ASN		34.050		12.434		32.98
ATOM		L CB	ASN		35.198		11.114	1.00	34.97
ATOM	1 2322	CG	ASN		36.540		10.541	1.00	39.89
ATOM		OD:	l ASN		37.044		11.103	1.00	45.37
ATOM	2324	ND2	2 ASN		37.125		10.826	1.00	48.43
ATOM	2327	C C	ASN		32.846	-15.141 -13.947	11.909	1.00	45.88
ATOM		0	ASN		32.646	-13.947	10.192	1.00	33.97
ATOM		N	GLU	1728	32.024	-14.973	9.341	1.00	35.07
ATOM		CA	GLU	1728	30.814	-15.210	10.414	1.00	31.69
ATOM		CB	GLU	1728	30.141	-16.493	9.620	1 00	30.27
ATOM		CG	GLU	1728	28.932	-16.878	10.083	1.00	32.53
ATOM		CD	GLU	1728	28.353	-18.190	9.273	1.00	32.81
ATOM	2335	OE1	GLU	1728	28.339	-18.190	9.711	1.00	36.43
MOTA	2336	OE2	GLU	1728	27.908	-18,945	10.932	1.00	36.75
ATOM	2337	C	GLU	1728	29.814	-14.049	8.829	1.00	41.92
ATOM	2338	0	GLU	1728	29.234	-13.655	9 681	1.00	28.70
ATOM	2339	N	LEU	1729	29.594	-13.517	8.660 10.880	1.00	28.51
ATOM	2341	CA	LEU	1729	28.687	-12.393	11.040	1.00	26.77
ATOM	2342	CB	LEU	1729	28.228	-12.274	12.490	1.00	26.80
ATOM	2343	CG	LEU	1729	27.233	-13.355	12.913	1.00	27.91
ATOM	2344	CD1	LEU	1729	27.095	-13.345	14.428	1.00 1.00	30.71
ATOM	2345	CD2	LEU	1729	25.885	-13.141	12.253		35.79
ATOM	2346	С	LEU	1729	29.319	-11.089	10.540	1.00	25.70
ATOM	2347	O	LEU	1729	28.610		10.126	_	27.06
ATOM	2348	N	TYR	1730	30.650		10.549	1.00	30.27
ATOM ATOM	2350	CA	TYR	1730	31.328		10.039		27.03
ATOM	2351	CB	TYR	1730	32.792		10.474		26.21 25.31
ATOM	2352	CG	TYR	1730	33.538	-8.553	9.982		23.31 24.89
ATOM	2353	CD1	TYR	1730	33.012	<b>.</b> .	10.169		23.59
ATOM	2354	CE1	TYR	1730	33.655	-6.148	9.665		23.59 24.74
	2355	CD2	TYR	1730	34.739	-8.675	9.285		
ATOM	2356	CE2	TYR	1730	35.399	-7.560	8.775		22.11 22.32
MOTA	2357	CZ	TYR	1730	34.853	-6.295			
ATOM	2358	ОН	TYR	1730	35.484	~5.181	_		26.07
ATOM ATOM	2360	C	TYR	1730	31.227	-9.878			22.70
	2361	0	TYR	1730	30.960	-8.875			27.71
ATOM	2362	N	MET	1731	31.409	-11.081			28.05 27.92
MOTA MOTA	2364	CA	MET	1731	31.306	-11.355			
	2365	CB	MET	1731	31.506	-12.853	_		8.89
ATOM	2366	CG	MET	1731	31.068	-13.379			5.84 5.50
ATOM ATOM	2367	SD	MET	1731	31.347				6.40
-1 OM	2368	CE	MET	1731					6.88
								5	0.00

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MOTA	2369	С	MET	1731	29.916	-10.928	6.102	1.00	27.79
ATOM	2370	0	MET	1731	29.755	-10.345	5.041	1.00	30.68
ATOM	2371	N	MET	1732	28.915	-11.203	6.932	1.00	28.02
MOTA	2373	CA	MET	1732	27.546	-10.804	6.639	1.00	25.74
MOTA	2374	CB	MET	1732	26.598	-11.317	7.718	1.00	24.94
MOTA	2375	CG	MET	1732	25.153	-10.911	7.492	1.00	22.96
ATOM	2376	SD	MET	1732	24.008	-11.593	8.684	1.00	24.39
ATOM	2377	CE	MET	1732	23.798	-13.272	8.002	1.00	18.04
ATOM	2378	C	MET	1732	27.470	-9.273	6.559	1.00	25.81
ATOM	2379	0	MET	1732	26.889	-8.729	5.620	1.00	26.85
ATOM	2380	N	MET	1733	28.068	-8.587	7.53.7	1.00	24.84
ATOM	2382	CA	MET	1733	28.092	-7.124	7.545	1.00	25.27
MOTA	2383	CB	MET	1733	28.931	-6.6.00	9.700	1.00	25.97
ATOM	2384	CG	MET	1733	28.342	-6.769	10.058	1.00	28.69
MOTA	2385	SD	MET	1733	29.456	-6.094	11.295	1.00	29.06
ATOM	2386	CE	MET	1733	28.927	-7.051	12.693	1.00	28.07
ATOM	2387	С	MET	1733	28.741	-6.628	6.270	1.00	26.97
ATOM	2388	0	MET	1733	28.192	-5.771	5.581	1.00	28.37
ATOM	2389	N	ARG	1734	29.922	-7.160	5.966	1.00	28.77
ATOM	2391	CA	ARG	1734	30.664	-6. <b>7</b> 75	4.762	1.00	29.66
MOTA	2392	CB	ARG	1734	32.027	-7.482	4.716	1.00	29.05
MOTA	2393	CG	ARG	1734	32.968	-7.109	5.866	1.00	25.00
MOTA	2394	CD	ARG	1734	33.247	-5.621	5.882	1.00	29.27
MOTA	2395	NE	ARG	1734	33.911	-5.210	4.647	1.00	35.43
MOTA	2397	cz	ARG	1734	35.233	-5.220	4.466	1.00	38.24
ATOM	2398	NH1	ARG	1734	36.054	-5.601	5.445	1.00	36.47
MOTA	2401	NH2	ARG	1734	35.732	-4.907	3.277	1.00	38.57
ATOM	2404	C	ARG	1734	29.859	-7.034	3.478	1.00	29.57
MOTA	2405	0	ARG	1734	29.920	-6.242	2.538	1.00	29.55
MOTA	2406	N	ASP	1735	29.095	-8.124	3.448	1.00	28.07
MOTA	2408	CA	ASP	1735	28.259	-8.423	2.287	1.00	27.96
MOTA	2409	CB	ASP	1735	27.634	-9.813	2.408	1.00	28.60
MOTA	2410	CG	ASP	1735	28.664	-10.926	2.283	1.00	31.34
MOTA	2411	OD1	ASP	1735	29.785	-10.660	1.798	1.00	31.12
ATOM	2412	OD2	ASP	1735	28.356	-12.068	2.687	1.00	36.07
MOTA	2413	С	ASP	1735	27.159	-7.368	2.155	1.00	27.24
ATOM	2414	0	ASP	1735	26.846	-6.932	1.050	1.00	25.79
ATOM	2415	N	CYS	1736	26.590	-6.951	3.288	1.00	26.53
ATOM	2417	CA	CYS	1736	25.547	-5.930	3.314	1.00	24.35
ATOM	2418	CB	CYS	1736	24.968	-5.765	4.731	1.00	22.01
ATOM	2419	SG	CYS	1736	23.885	-7.101	5.281	1.00	21.52
MOTA	2420	C	CYS	1736	26.119	-4.595	2.847	1.00	24.26
ATOM	2421	0	CYS	1736	25.386	-3.725	2.368	1.00	24.19
ATOM	2422	N	TRP	1737	27.432	-4.437	3.002	1.00	22.94
ATOM	2424	CA	TRP	1737	28.104	-3.210	2.605	1.00	21.91
ATOM	2425	CB	TRP	1737	29.146	-2.820	3.640	1.00	19.26
ATOM	2426	CG	TRP	1737	28.572	-2.493	4.947	1.00	20.89
ATOM	2427	CD2	TRP	1737	29.226	-2.602	6.212	1.00	23.33
ATOM	2428	CE2	TRP	1737	28.315	-2.159	7.196	1.00	21.59
ATOM	2429	CE3	TRP	1737	30.506	-3.026	6.614	1.00	25.00
ATOM	2430	CD1	TRP	1737	27.319	-2.012	5.201	1.00	19.90
ATOM	2431	NEl	TRP	1737	27.158	-1.807	6.551	1.00	20.77
ATOM	2433	CZ2	TRP	1737	28.641	-2.127	8.563	1.00	19.89
MOTA	2434	CZ3	TRP	1737	30.825	-2.993	7.971	1.00	21.23



ATO			2 TRI	1737	29.896	-2.54	8.92	7 1 00	) 21 0/
ATO		6 C	TRI	2 1737	28.758				
ATO	M 243°	7 0	TRE	1737	29.653				
ATO		3 N	HIS	1738	28.315				
MOTA		CA	HIS		28.877				
ATON		CB	HIS		28.243	,			
NOTA	1 2442	CG	HIS		29.131				
ATOM	1 2443	CD2			29.595				
MOTA	1 2444	ND1	HIS		29.681				
ATOM	1 2446	CE1	HIS		30.436	_			
ATOM	2447	NE2	HIS		30.409				
ATOM	2449	C	HIS		28.716	-6.358			
ATOM	2450	0	HIS		27.675	-2.970		1.00	25.82
ATOM	2451	N	ALA		29.802	-2.314	-1.660	1.00	23.96
ATOM	2453	CA	ALA	1739	29.825	-2.564	-2.362	1.00	26.27
ATOM	2454	CB	ALA	1739	31.186	-1.346	-3.158	1.00	25.46
ATOM	2455	С	ALA	1739	28.754	-1.180	-3.789	1.00	25.70
ATOM	2456	0	ALA	1739	28.116	-1.443	-4.233	1.00	26.18
ATOM	2457	N	VAL	1740	28.570	-0.455	-4.574	1.00	29.14
ATOM	2459	CA	VAL	1740	27.560	-2.643	-4.774	1.00	25.71
ATOM	2460	СВ	VAL	1740	28.063	-2.875	-5.802	1.00	26.12
ATOM	2461	CG1	VAL	1740	27.102	-3.841	-6.903	1.00	25.99
ATOM	2462	CG2	VAL	1740	29.450	-3.832	-8.090	1.00	23.37
ATOM	2463	C	VAL	1740	26.247	-3.440	-7.349	1.00	22.07
ATOM	2464	0	VAL	1740	26.247	-3.400	-5.191	1.00	25.43
ATOM	2465	N	PRO	1741	25.170	-4.550	-4.704	1.00	24.93
ATOM	2466	CD	PRO	1741	25.170	-2.585	-5.265	1.00	24.20
ATOM	2467	CA	PRO	1741	23.131	-1.277	-5.953	1.00	18.88
ATOM	2468	CB	PRO	1741	22.953	-2.914	-4.734	1.00	25.28
MOTA	2469	CG	PRO	1741	23.903	1.788	-5.294	1.00	22.75
MOTA	2470	C	PRO	1741	23.299	-0.632	-5.398	1.00	20.99
MOTA	2471	O	PRO	1741	22.787	-4.296 -F.036	-5.128	1.00	25.84
MOTA	2472	N.	SER	1742	23.425	-5.036	-4.280	1.00	25.99
ATOM	2474	CA	SER	1742	22.942	-4.642 -5.010	-6.407	1.00	26.48
MOTA	2475	СВ	SER	1742	23.151	-5.919	-6.930	1.00	25.19
MOTA	2476	OG	SER	1742	24.530	-5.992 -5.943	-8.440	1.00	25.68
ATOM	2478	С	SER	1742	23.644	-5.943	-8.769	1.00	27.46
ATOM	2479	0	SER	1742	23.124	-7.100	-6.289	1.00	25.24
ATOM	2480	N	GLN	1743	24.826	-8.218	-6.300	1.00	26.09
ATOM	2482	CA	GLN	1743	25.590	-6.851 -7.917	-5.731	1.00	23.88
ATOM	2483	CB	GLN	1743	27.069	-7.733	-5.118	1.00	24.44
ATOM	2484	CG	GLN	1743	27.344	-7.784	-5.437	1.00	27.26
ATOM	2485	CD	GLN	1743	26.803		-6.940	1.00	27.39
MOTA	2486	OE1	GLN	1743	27.325	-9.047 -10.136	-7.581	1.00	26.46
MOTA	2487	NE2	GLN	1743	25.760		-7.339	1.00	25.80
ATOM	2490	С	GLN	1743	25.348	-8.914	-8.393	1.00	27.42
ATOM	2491	0	GLN	1743	25.810	-8.151	-3.633	1.00	23.20
ATOM	2492	N	ARG	1744		-9.147	-3.083	1.00	22.90
MOTA	2494	CA	ARG	1744	24.628 24.318	-7.243	-2.984	1.00	22.15
ATOM	2495	CB	ARG	1744	23.767	-7.398	-1.568	1.00	21.23
ATOM	2496	CG	ARG	1744	24.705	-6.088	-0.998	1.00	19.01
ATOM	2497	CD		1744	24.703	-4.916	-1.145	1.00	17.27
ATOM	2498	NE		1744	24.091	-3.605	-0.679	1.00	14.79
ATOM	2500			1744		-2.493	*		19.72
				- / 77	24.482	-1.258	-1.391	1.00	19.23

ATOM	2501	NHl	ARG	1744	23.201	-0.931	-1.201	1.00	15.90
MOTA	2504	NH2	ARG	1744	25.343	-0.343	-1.821	1.00	19.43
ATOM	2507	C	ARG	1744	23.259	-8.496	-1.438	1.00	21.95
ATOM	2508	0	ARG	1744	22.585	-8.827	-2.415	1.00	25.34
ATOM	2509	N	PRO	1745	23.213	-9.184	-0.292	1.00	20.82
ATOM	2510	CD	PRO	1745	24.191	-9.219	0.804	1.00	21.25
MOTA	2511	CA	PRO	1745	22.204	-10.229	-0.127	1.00	21.39
MOTA	2512	CB	PRO	1745	22.687	-10.980	1.117	1.00	21.69
MOTA	2513	CG	PRO	1745	23.418	-9. <b>9</b> 16	1.886	1.00	22.62
MOTA	2514	С	PRO	1745	20.833	-9.585	0.102	1.00	22.15
MOTA	2515	0	PRO	1745	20.739	-8.402	0.426	1.00	23.29
MOTA	2516	N	THR	1746	19.771	-10.349	-0.109	1.00	20.93
ATOM	2518	CA	THR	1746	18.440	-9.827	0.107	1.00	19.90
ATOM	2519	CB	THR	1746	17.391	-10.554	-0.783	1.00	20.21
ATOM	2520	OG1	THR	1746	17.484	-11.974	-0.584	1.00	22.03
ATOM	2522	CG2	THR	1746	17.609	-10.242	-2.255	1.00	20.82
MOTA	2523	C	THR	1746	18.112	-10.095	1.557	1.00	19.77
MOTA	2524	0	THR	1746	18.842	-10.823	2.228	1.00	19.19
ATOM	2525	N	PHE	1747	17.010	-9.526	2.045	1.00	23.46
ATOM	2527	CA	PHE	1747	16.582	-9.770	3.422	1.00	21.64
ATOM	2528	CB	PHE	1747	15.473	-8.794	3.827	1.00	18.69
MOTA	2529	CG	PHE	1747	15.987	-7.445	4.262	1.00	17.45
ATOM	2530	CD1	PHE	1747	16.757	-7.317	5.417	1.00	17.65
ATOM	2531	CD2	PHE	1747	15.712	-6.303	3.516	1.00	15.37
ATOM	2532	CE1	PHE	1747	17.242	-6.073	5.819	1.00	16.17
ATOM	2533	CE2	PHE	1747	16.189	-5.056	3.907	1.00	14.53
ATOM	2534	CZ	PHE	1747	16.959	-4.941	5.065	1.00	16.98
MOTA	2535	С	PHE	1747	16.118	-11.227	3.522	1.00	23.18
ATOM	2536	0	PHE	1747	16.271	-11.873	4.548	1.00	24.04
MOTA	2537	N	LYS	1748	15.570	-11.745	2.432	1.00	24.13
ATOM	2539	CA	LYS	1748	15.137	-13.132	2.385	1.00	26.35
ATOM	2540	CB	LYS	1748	14.502	-13.424	1.024	1.00	27.52
ATOM	2541	CG	LYS	1748	14.034	-14.849	0.836	1.00	33.88
ATOM	2542	CD	LYS	1748	13.598	-15.062	-0.600	1.00	41.83
MOTA	2543	CE	LYS	1748	13.190	-16.506	-0.881	1.00	50.05
MOTA	2544	NZ	LYS	1748	12.084	-16.986	0.005	1.00	55.70
ATOM	2548	C	LYS	1748	16.359	-14.037	2.636	1.00	27.50
MOTA	2549	0	LYS	1748	16.303	-14.950	3.459	1.00	31.18
ATOM	2550	N	GLN	1749	17.467	-13.761	1.949	1.00	27.24
ATOM	2552	CA	GLN	1749	18.699	-14.529	2.122	1.00	27.03
MOTA	2553	CB	GLN	1749	19.797	-14.039	1.169	1.00	31.80
ATOM	2554	CG	GLN	1749	19.501	-14.196	-0.323	1.00	38.57
ATOM	2555	CD	GLN	1749	20.460	-13.385	-1.209	1.00	39.93
MOTA	2556	OE1	GLN	1749	20.025	-12.535	-1.974	1.00	39.90
ATOM	2557	NE2	GLN	1749	21.768	-13.620	-1.068	1.00	40.23
MOTA	2560	C	GLN	1749	19.205	-14.380	3.552	1.00	25.98
MOTA	2561	0	GLN	1749	19.533	-15.371	4.198	1.00	27.18
ATOM	2562	N	LEU	1750	19.293	-13.133	4.018	1.00	25.20
MOTA	2564	CA	LEU	1750	19.774	-12.823	5.369	1.00	25.74
ATOM	2565	CB	LEU	1750	19.722	-11.317	5.631	1.00	20.99
ATOM	2566	CG	LEU	1750	20.708	-10.468	4.831	1.00	20.90
ATOM	2567	CD1	LEU	1750	20.302	-8.987	4.822	1.00	19.88
MOTA	2568	CD2	LEU	1750	22.071	-10.643	5.426	1.00	17.26
MOTA	2569	C	LEU	1750	18.985	-13.555	6.441	1.00	27.10



ATON	1 2570								
ATOM			LEU		19.553			1.00	27.89
ATOM			VAL		17.672			-	29.40
ATOM			VAL		16.798		•	1.00	26.80
ATOM		_	VAL		15.324			1.00	
ATOM					14.429			1.00	29.93
ATOM					14.941		7.117	1.00	24.10
ATOM		_	VAL		17.136		7.228	1.00	27.80
ATOM			VAL		17.223	-	8.285		26.77
ATOM			GLU	1752	17.408	-16.300	6.056	1.00	32.26
ATOM			GLU	1752	17.749	~17.717	5.966	1.00	35.72
ATOM		CB	GLU	1752	17.721	-18.173	4.504	1.00	39.33
ATOM		CG	GLU		16.306	-18.078	3.911	1.00	49.41
ATOM		CD	GLU	1752	16.209	-18.421	2.429	1.00	55.88
ATOM	2585	OE1	GLU	1752	15.141	-18.138	1.835	1.00	58.00
ATOM	2586	OE2	GLU	1.752	17.180	-18.978	1.863	1.00	61.03
ATOM	2587	C	GLU	1752	19.093	-18.002	6.635	1.00	34.59
ATOM	2588	0	GLU	1752	19.230	-18.975	7.393	1.00	33.95
ATOM	2589	Ŋ	ASP	1753	20.057	-17.114	6.401	1.00	34.38
ATOM	2591	CA	ASP	1753	21.393	-17.235	6.977	1.00	32.81
ATOM	2592	CB	ASP	1753	22.338	-16.227	6.334	1.00	31.57
ATOM	2593	CG	ASP	1753	22.628	-16.556	4.888	1.00	33.68
	2594	OD1	ASP	1753	22.573	-17.755	4.536	1.00	35.14
MOTA MOTA	2595	OD2	ASP	1753	22.914	-15.624	4.104	1.00	34.44
ATOM	2596	C.	ASP	1753	21.378	-17.058	8.489	1.00	32.04
ATOM	2597	0	ASP	1753	21.997	-17.837	9.214	1.00	31.21
MOTA	2598	N	LEU	1754	20.648	-16.045	8.955	1.00	31.00
ATOM	2600	CA	LEU	1754	20.528	-15.754	10.382	1.00	29.46
ATOM	2601	CB	LEU	1754	19.822	-14.426	10.598	1.00	23.47
ATOM	2602	CG	LEU	1754	20.816	-13.309	10.318	1.00	23.58
ATOM	2603	CD1	LEU	1754	20.114	-11.963	10.128	1.00	20.46
ATOM	2604	CD2	LEU	1754	21.828	-13.282	11.462	1.00	19.18
ATOM	2605	C	LEU	1754	19.806	-16.866	11.110	1.00	31.84
ATOM	2606	0	LEU	1754	20.125	-17.178	12.254	1.00	30.78
ATOM	2607 2609	И	ASP	1755	18.832	-17.471	10.445	1.00	34.03
ATOM	2610	CA	ASP	1755	18.116	-18.578	11.044	1.00	35.22
ATOM	2611	CB	ASP	1755	16.973	-19.027	10.148	1.00	38.40
ATOM	2612	CG	ASP	.1755	16.159	-20.119	10.779	1.00	41.85
ATOM	2612	OD1	ASP	1755	15.560	-19.866	11.841	1.00	47.90
ATOM	2613	OD2	ASP	1755	16.142	-21.241	10.238	1.00	46.67
ATOM	2615	C	ASP	1755	19.114	-19.724	11.222	1.00	36.79
ATOM	2616	C	ASP	1755	19.114	-20.411	12.250	1.00	38.33
ATOM		N	ARG	1756	19.973	-19.920	10.226	1.00	34.81
ATOM	2618	CA	ARG	1756	20.982	-20.969	10.302	1.00	34.68
ATOM	2619	CB	ARG	1756	21.688	-21.100	8.959	1.00	34.78
ATOM	2620	CG	ARG	1756	22.746	-22.179	8.910	1.00	35.93
MOTA	2621	CD	ARG	1756	23.297	-22.306	7.511	1.00	41.60
ATOM	2622	NE	ARG	1756	23.786	-21.025	6.999	1.00	46.42
	2624	CZ	ARG	1756	24.889	-20.419	7.427	1.00	48.38
ATOM	2625	NH1	ARG	1756	25.637	-20.976	8.381	1.00	48.10
ATOM	2628	NH2	ARG	1756	25.236	-19.242	6.909	1.00	46.62
ATOM	2631	C	ARG	1756	22.002	-20.666	11.399	1.00	36.17
ATOM	2632	0	ARG	1756	22.372	-21.541	12.177	1.00	38.33
ATOM ATOM	2633	N	ILE	1757	22.433	-19.413	11.478	1.00	37.00
ATOM	2635	CA	ILE	1757	23.416	-18.998	12.468	1.00	35.60



ATOM	2636	CB	ILE	1757	23.964	-17.588	12.141	1.00	35.54
MOTA	2637	CG2	ILE	1757	24.921	-17.131	13.217	1.00	32.41
ATOM	2638	CG1	ILE	1757	24.693	-17.612	10.794	1.00	33. <b>7</b> 7
MOTA	2639	CD1	ILE	1757	25.097	-16.253	10.287	1.00	33.49
MOTA	2640	C	ILE	1757	22.866	-19.048	13.891	1.00	37.28
ATOM	2641	0	ILE	1757	23.531	-19.556	14.779	1.00	38.42
ATOM	2642	N	VAL	1758	21.634	-18.585	14.088	1.00	39.19
ATOM	2644	CA	LAV	1758	21.016	-18.584	15.421	1.00	39.84
MOTA	2645	CB	VAL	1758	19.560	-18.017	15.403	1.00	37.62
MOTA	2646	CG1	VAL	1758	18.918	-18.144	16.773	1.00	38.30
MOTA	2647	CG2	VAL	1758	19.560	-16.560	15.009	1.00	39.62
ATOM	2648	С	VAL	1758	20.983	-19.997	15.988	1.00	41.98
ATOM	2649	0	VAL	1758	21.380	-20.229	17.128	1.00	43.36
ATOM	2650	N	ALA	1759	20.501	-20.932	15.182	1.00	43.31
ATOM	2652	C'A	ALA	1759	20.418	-22.325	15.589	1.00	44.00
MOTA	2653	CB	ALA	1759	19.836	-23.150	14.459	1.00	44.52
MOTA	2654	C	ALA	1759	21.784	-22.867	15.976	1.00	45.98
ATOM	2655	0	ALA	1759	21.894	-23.725	16.841	1.00	48.78
MOTA	2656	И	LEU	1760	22.823	-22.375	15.319	1.00	48.93
ATOM	2658	CA	LEU	1760	24.175	-22.831	15.592	1.00	51.47
ATOM	2659	CB	LEU	1760	24.954	-22.900	14.280	1.00	53.63
ATOM	2660	CG	LEU	1760	24.284	-23.864	13.295	1.00	57.84
MOTA	2661	CD1	LEU	1760	24.993	-23.847	11.948	1.00	61.83
ATOM	2662	CD2	LEU	1760	24.260	-25.277	13.886	1.00	58.57
ATOM	2663	C	LEU	1760	24.911	-21.965	16.607	1.00	53.60
ATOM	2664	0	LEU	1760	26.078	-22.214	16.919	1.00	54.00
MOTA	2665	JN	THR	1761	24.222	-20.963	17.141	1.00	55.77
ATOM	2667	CA	THR	1761	24.820	-20.060	18.111	1.00	56.64
ATOM	2668	CB	THR	1761	24.250	-18.627	17.979	1.00	55.76
ATOM	2669	OG1	THR	1761	24.444	-18.154	16.644	1.00	56.20
ATOM	2671	CG2	THR	1761	24.962	-17.680	18.917	1.00	55.25
ATOM	2672	C	THR	1761	24.636	-20.548	19.539	1.00	58.16
MOTA MOTA	2673	0	THR	1761	23.566	-21.021	19.919	1.00	56.85
	2674	N	SER	1762	25.706	-20.436	20.318	1.00	61.74
ATOM ATOM	2676 2677	CA CB	SER	1762	25.706	-20.833	21.717	1.00	64.50
ATOM	2678		SER	1762	27.155	-20.979	22.205	1.00	68.82
ATOM	2680	OG C	SER	1762	27.232	-21.544	23.508	1.00	73.15
ATOM	2681	0	SER SER	1762 1762	24.965	-19.775	22.547	1.00	63.87
ATOM	3420	PA	PCP	400	25.080 62.748	-18.563 10.301	22.296	1.00	63.22
ATOM	3421	O1A	PCP	400	62.509	10.301	7.817 9.280	1.00	90.90
ATOM	3422	02A	PCP	400	61.832	11.180	7.038	1.00	92.35
ATOM	3423	05*	PCP	400	62.744	8.904	7.142	1.00	90.49 83.57
ATOM	3424	PB	PCP	400	65.226	11.946	8.294	1.00	
ATOM	3425	OlB	PCP	400	65.246	13.015	7.264	1.00	101.51 102.85
ATOM	3426	02B	PCP	400	66.527	11.458	8.830	1.00	
ATOM	3427	03A	PCP	400	64.334	10.725	7.584	1.00	99.88
ATOM	3428	C3B	PCP	400	64.345	12.502	9.635		96.64
ATOM	3429	C5.*	PCP	400	62.337	8.684	5.839	1.00	102.94 71.21
ATOM	3430	C4 *	PCP	400	62.337	7.204	5.587	1.00	71.21 64.48
ATOM	3431	04 *	PCP	400	63.713	6.745	6.169	1.00	60.91
ATOM	3432	C1*	PCP	400	63.394	5.459	6.680	1.00	54.96
ATOM	3433	N9	PCP	400	64.326	5.101	7.712	1.00	47.26
ATOM	3434	C4	PCP	400	65.017	3.903	7.712	1.00	46.24
					05.017	5.503	/ . O T	1.00	70.24

ATOM	1 3435	5 N3	PCI	400	64.926	2.770	7.062	1.00	43.00
ATOM		5 C2	PCI	400	65.802	1.878			
ATOM	3437	7 N1	PCF	400	66.674	1.917			
ATOM		3 C6	PCF	400	66.735	3.028			
ATOM		9 N6	PCF	400	67.573	3.134			
ATOM	3442	C5	PCF	400	65.862	4.091		-	
ATOM	3443	N7	PCP	400	65.674	5.361			
MOTA		C8	PCP	400	64.761	5.894		1.00	
ATOM	3445	C2*	PCP	400	61.986	5.500		1.00	
ATOM		02*	PCP	400	61.454	4.153	7.234	1.00	57.63
ATOM	3448	C3 *	PCP		61.328	6.402	6.245	1.00	56.45
MOTA	3449	03*	PCP	400	60.689	5.644	5.206	1.00	61.31
ATOM	3451	PA	PCP	401	9.366	9.801	17.743	1.00	64.65
ATOM	3452	Ola	PCP	401.	9.463	8.736	16.709	0.50	74.43
ATOM	3453	02A	PCP	401	10.330	10.926	17.699	0.50	75.37
ATOM	3454	05*	PCP	401	9.427	9.108	19.186	0.50	75.86
ATOM	3455	PB	PCP	401	6.878	10.679	16.547	0.50	67.44
ATOM	3456	Olb	PCP	401	6.223	11.982	16.778	0.50	82.27
ATOM	3457	02B	PCP	401	6.020	9.486	16.408	0.50	82.91
ATOM	3458	<b>A</b> EO	PCP	401	7.868	10.423	17.814	0.50	82.70
ATOM	3459	C3B	PCP	401	7.790	10.845	15.159	0.50	78.30
ATOM	3460	C5*	PCP	401	10.184	9.593	20.275	0.50	82.50
MOTA	3461	C4*	PCP	4.01	10.228	8.637	21.442	0.50 0.50	54.44
ATOM	3462	04*	PCP	401	9.032	7.855	21.412		45.38
ATOM	3463	C1*	PCP	401	9.397	6.509	21.412	0.50 0.50	39.40
ATOM	3464	N9	PCP	401	8.386	5.627	21.044	0.50	35.00
ATOM	3465	C4	PCP	401	7.790	4.469	21.564	0.50	27.91
ATOM	3466	N3	PCP	401	7.982	3.849	22.732	0.50	23.36 22.33
ATOM	3467	C2	PCP	401	7.239	2.768	22.838	0.50	
ATOM	3468	N1	PCP	401	6.382	2.251	22.003	0.50	20.26 17.29
ATOM	3469	C6	PCP	401	6.202	2.877	20.856	0.50	19.35
ATOM	3470	N6	PCP	401	5.327	2.415	19.975	0.50	16.87
ATOM	3473	C5	PCP	401	6.932	4.038	20.603	0.50	21.72
ATOM	3474	N7	PCP	401	6.983	4.880	19.507	0.50	24.59
ATOM	3475	C8	PCP	401	7.847	5.786	19.832	0.50	24.26
MOTA	3476	C2*	PCP	401	10.762	6.409	20.931	0.50	39.01
ATOM	3477	02*	PCP	401	11.609	5.326	21.412	0.50	43.88
ATOM	3479	C3*	PCP	401	11.396	7.674	21.373	0.50	42.14
ATOM	3480	03*	PCP	401	11.918	7.515	22.681	0.50	44.21
ATOM	3482	N	SER	461	78.844	26.057	14.057	1.00	43.87
ATOM	3484	CA	SER	461	79.399	24.884	13.385	1.00	43.50
ATOM	3485	CB	SER	461	78.488	23.655	13.616	1.00	39.99
ATOM	3486	C	SER	461	79.572	25.181	11.888	1.00	42.14
ATOM	3487	0	SER	461	79.473	24.292	11.038	1.00	40.29
ATOM	3488	N	GLU	462	79.883	26.441	11.594	1.00	43.19
ATOM	3490	CA	GLU	462	80.061	26.951	10.233	1.00	42.77
ATOM	3491	CB	GLU	462	80.303	28.446	10.250	1.00	47.75
ATOM	3492	CG	GLU	462	79.209	29.301	10.860	1.00	60.57
ATOM	3493	CD	GLU	462	79.647	30.752	11.061	1.00	67.56
ATOM	3494	OE1	GLU	462	80.866	31.016	10.994		67.47
ATOM	3495	OE2	GLU	462	78.764	31.611			72.32
ATOM	3496	C	GLU	462	81.207	26.357	9.457		39.55
MOTA	3497	0	GLU	462	81.051	26.032		1.00	38.74
ATOM	3498	N	TYR	463	82.375	26.299		1.00	36.47

ATOM	3500	CA	TYR	463	83.567	25.806	9.420	1.00	34.19
ATOM	3501	CB	TYR	463	84.702	26.828	9.505	1.00	35.55
MOTA	3502	CG	TYR	463	84.393	28.059	8.675	1.00	42.11
MOTA	3503	CD1	TYR	463	84.004	29.264	9.283	1.00	43.15
ATOM	3504	CE1	TYR	463	83.619	30.361	8.513	1.00	42.40
ATOM	3505	CD2	TYR	463	84.395	27.990	7.280	1.00	3,9.78
MOTA	3506	CE2	TYR	463	84.012	29.078	6.509	1.00	39.04
ATOM	3507	CZ	TYR	463	83.625	30.256	7.129	1.00	39.86
MOTA	3508	OH	TYR	463	83.260	31.330	6.366	1.00	42.58
ATOM	3510	C	TYR	463	84.055	24.434	9.800	1.00	33.28
ATOM	3511	0	TYR	463	84.739	23.781	9.005	1.00	33.47
· ATOM	3512	N	GLU	464	83.695	23.976	10.993	1.00	34.42
ATOM	3514	CA	GLU	464	84.117	22.660	11.444	1.00	36.38
ATOM	3515	CB	GLU	464	85.618	22.663	11.750	1.00	40.90
MOTA	3516	CG	GLU	464	86.041	23.755	12.729	1.00	46.29
MOTA	3517	CD	GLU	464	87.548	23.810	12.943	1.00	51.33
MOTA	3518	OEl	GLU	464	87.970	24.247	14.038	1.00	54.49
ATOM	3519	OE2	GLU	464	88.312	23.430	12.025	1.00	53.18
MOTA	3520	С	GLU	464	83.374	22.224	12.678	1.00	35.64
MOTA	3521	O	GLU	464	83.111	23.052	13.555	1.00	37.40
MOTA	3522	N	LEU	465	82.962	20.955	12.711	1.00	34.21
ATOM	3524	CA	LEU	465	82.267	20.429	13.887	1.00	34.92
ATOM	3525	CB	LEU	465	81.285	19.300	13.542	1.00	31.30
ATOM	3526	CG	LEU	465	80.272	19.381	12.405	1.00	32.22
ATOM	3527	CD1	LEU	465	79.152	18.407	12.720	1.00	21.95
ATOM	3528	CD2	LEU	465	79.738	20.802	12.212	1.00	29.75
ATOM	3529	C	LEU	465	83.326	19.855	14.814	1.00	36.17
ATOM	3530	0	LEU	465	84.473	19.621	14.400	1.00	35.80
MOTA	3531	N	PRO	466	82.970	19.629	16.083	1.00	36.20
ATOM	3532	CD	PRO	466	81.722	20.018	16.758	1.00	38.17
ATOM	3533	CA	PRO	466	83.925	19.072	17.037	1.00	36.06
ATOM	3534	СВ	PRO	466	83.132	19.035	18.333	1.00	35.57
MOTA	3535	CG	PRO	466	82.185	20.194	18.171	1.00	38.67
MOTA	3536	С	PRO	466	84.294	17.666	16.605	1.00	37.06
ATOM	3537	0	PRO	466	83.498	16.959	15.979	1.00	34.50
ATOM	3538	N	GLU	467	85.504	17.258	16.936	1.00	39.97
MOTA	3540	CA	GLU	467	85.951	15.932	16.587	1.00	44.69
MOTA	3541	CB	GLU	467	87.412	15.985	16.151	1.00	50.43
MOTA	3542	CG	GLU	467	87.902	14.695	15.518	1.00	60.27
MOTA	3543	CD	GLU	467	89.321	14.796	14.986	1:00	65.75
MOTA	3544	OE1	GLU	467	90.024	15.804	15.269	1.00	64.40
ATOM	3545	OE2	GLU	467	89.726	13.850	14.275	1.00	71.13
ATOM	3546	С	GLU	467	85.775	15.002	17.783	1.00	43.30
ATOM	3547	0	GLU	467	85.888	15.428	18.936	1.00	43.26
ATOM	3548	N	ASP	468	85.433	13.750	17.504	1.00	43.09
ATOM	3550	CA	ASP	468	85.254	12.739	18.545	1.00	44.15
MOTA	3551	CB	ASP	468	83.785	12.614	18.979	1.00	44.54
ATOM	3552	CG	ASP	468	83.574	11.562	20.072	1.00	41.84
ATOM	3553	OD1	ASP	468	82.405	11.244	20.368	1.00	39.81
ATOM	3554	OD2	ASP	468	84.570	11.057	20.636	1.00	42.92
MOTA	3555	C	ASP	468	85.746	11.422	17.970	1.00	44.66
ATOM	3556	ō	ASP	468	84.982	10.663	17.368	1.00	44.56
ATOM	3557	N	PRO	469	87.034	11.126	18.176	1.00	44.56
ATOM	3558	CD	PRO	469	87.953	11.959	18.971	1.00	45.43
					J., J.J.J		40.91L	1.00	7J.4J



ATOM		CA	PRO	469	87.707	9.916	17.707	1.00	43.90
ATOM		CB	PRO	469	89.024	9.959	18.476	1.00	45.66
ATOM	3561	CG	PRO	469	89.300	11.438	18.547	1.00	44.89
ATOM	3562	C	PRO	469	86.934	8.627	17.971	1.00	42.60
MOTA	3563	0	PRO	469	86.935	7.730	17.139	1.00	41.35
MOTA	3564	N	ARG	470	86.229	8.569	19.096	1.00	43.25
ATOM	3566	CA	ARG	470	85.460	7.380	19.470	1.00	
ATOM	3567	CB	ARG	470	84.722	7.612	20.789	1.00	44.81
ATOM	3568	CG	ARG	470	85.579	8.201	21.889		48.36
ATOM	3569	CD	ARG	470	84.764	8.458	23.138	1.00	53.41
ATOM	3570	NE	ARG	470	83.581	9.261	22.861	1.00	55.42
ATOM	3572	CZ	ARG	470	82.748	9.712	23.791	1.00	58.57
ATOM	3573	NH1	ARG	470	82.972	9.445	25.077	1.00	62.24
ATOM	3576	NH2	ARG	470	81.670	10.398		1.00	64.57
ATOM	3579	C	ARG	470	84.439	6.924	23.436	1.00	63.66
ATOM	3580	0	ARG	470	84.166		18.437	1.00	43.69
ATOM	3581	N	TRP	471	83.879	5.735	18.313	1.00	45.68
ATOM	3583	CA	TRP	471	82.851	7.866	17.693	1.00	42.41
ATOM	3584	CB	TRP	471		7 534	16.720	1.00	38.92
ATOM	3585	CG	TRP	471	81.577	8.268	17.095	1.00	35.80
ATOM	3586	CD2	TRP	471	80.967	7.741	18.335	1.00	37.13
ATOM	3587	CE2	TRP	471	80.158	6.569	18.443	1.00	37.26
ATOM	3588	CE3			79.723	6.483	19.785	1.00	38.20
ATOM	3589	CD1	TRP TRP	471	79.748	5.582	17.530	1.00	35.59
ATOM	3590	NE1		471	81.010	8.300	19.584	1.00	36.42
ATOM	3592		TRP	471	80.260	7.553	20.462	1.00	35.89
ATOM		CZ2	TRP	471	78.896	5.454	20.239	1.00	36.18
ATOM	3593 3594	CZ3	TRP	471	78.934	4.561	17.978	1.00	32.81
ATOM	3594	CH2	TRP	471	78.514	4.505	19.321	1.00	34.82
ATOM		C	TRP	471	83.175	7.845	15.277	1.00	39. <b>7</b> 7
ATOM	3596	0	TRP	471	82.478	7.391	14.362	1.00	39.56
ATOM	3597	N	GLU	472	84.224	8.628	15.075	1.00	39.37
ATOM	3599	CA	GLU	472	84.605	9.043	13.739	1.00	38.42
ATOM	3600	CB	GLU	472	85.794	9.994	13.812	1.00	37.11
ATOM	3601	CG	GLU	472	85.958	10.849	12.582	1.00	34.11
	3602	CD	GLU	472	84.772	.11.757	12.338	1.00	34.03
ATOM	3603	OE1	GLU	472	84.260	12.348	13.317	1.00	31.87
ATOM	3604	OE2	GLU	472	84.367	11.885	11.163	1.00	32.11
ATOM	3605	С	GLU	472	84.910	7.901	12.791	1.00	39.78
MOTA	3606	0	GLU	472	85.656	6.975	13.128	1.00	41.64
ATOM	3607	N	LEU	473	84.303	7.958	11.610	1.00	37.71
ATOM	3609	CA	LEU	473	84.538	6.957	10.590	1.00	36.94
ATOM	3610	CB	LEU	473	83.258	6.196	10.265	1.00	35.38
MOTA	3611	CG	LEU	473	83.438	5.065	9.236	1.00	37.67
ATOM	3612	CD1	LEU	473	84.070	3.845	9.903	1.00	37.28
ATOM	3613	CD2	LEU	473	82.106	4.687	8.598	1.00	37.87
ATOM	3614	С	LEU	473	85.035	7.664	9.330	1.00	39.31
MOTA	3615	0	LEU	473	84.484	8.697	8.938	1.00	40.55
MOTA	3616	N	PRO	474	86.140	7.164	8.732	1.00	39.20
MOTA	3617	CD	PRO	474	87.052	6.170	9.327	1.00	37.83
MOTA	3618	CA	PRO	474	86.735	7.716	7.513	1.00	38.53
ATOM	3619	СВ	PRO	474	87.914	6.777	7.282	1.00	
ATOM	3620	CG	PRO	474	88.355	6.488	8.644	1.00	37.16
ATOM	3621	C	PRO	474	85.733	7.607	6.370	1.00	34.42
ATOM	3622	0	PRO	474	85.220	6.523			40.25
		-		- · -	03.220	0.523	6.098	1.00	40.70

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ATOM	3623	N	ARG	475	85.492	8.723	5.685	1.00	41.09
ATOM	3625	CA	ARG	475	84.534	8.746	4.590	1.00	42.26
MOTA	3626	CB	ARG	475	84.487	10.132	3.948	1.00	39.19
ATOM	3627	CG	ARG	475	83.957	11.199	4.876	1.00	35.19
ATOM	3628	CD	ARG	475	84.074	12.593	4.301	1.00	30.76
MOTA	3629	NE	ARG	475	83.796	13.567	5.345	1.00	22.86
MOTA	3631	CZ	ARG	475	82.581	13.898	5.748	1.00	21.99
MOTA	3632	NH1	ARG	475	81.529	13.350	5.165	1.00	23.39
ATOM	3635	NH2	ARG	475	82.412	14.662	6.813	1.00	22.55
ATOM	3638	С	ARG	475	84.838	7.692	3.538	1.00	45.38
ATOM	3639	0	ARG	475	83.927	7.182	2.892	1.00	47.15
MOTA	3640	N	ASP	476	86.106	7.319	3.390	1.00	47.13
ATOM	3642	CA	ASP	476	86.461	6.325	2.387	1.00	51.33
ATOM	3643	CB	ASP	476	87.973	6.294	2.134	1.00	55.23
ATOM	3644	CG	ASP	476	88.768	5.841	3.340	1.00	61.16
ATOM	3645	OD1	ASP	476	88.863	4.617	3.573	1.00	65.55
MOTA	3646	OD2	ASP	476	89.331	6.713	4.036	1.00	65.78
MOTA	3647	С	ASP	476	85.932 .	4.940	2.746	1.00	52.35
ATOM	3648	С	ASP	476	85.815	4.063	1.885	1.00	55.49
ATOM	3649	N	ARG	477	85.609	4.752	4.021	1.00	50.77
ATOM	3651	CA	ARG	477	85.080	3.482	4.508	1.00	48.65
ATOM	3652	CB	ARG	477	85.612	3.208	5.908	1.00	50.02
ATOM	3653	CG	ARG	477	8 <b>7</b> .067	2.799	5.881	1.00	55.33
ATOM	3654	CD	ARG	477	87.760	3.030	7.201	1.00	60.38
MOTA	3655	NE	ARG	477	87.238	2.207	8.285	1.00	64.36
ATOM	3657	CZ	ARG	477	87.748	2.203	9.513	1.00	69.16
ATOM	3658	NH1	ARG	477	88.794	2.968	9.814	1.00	70.73
ATOM	3661	NH2	ARG	477	87.190	1.459	10.159	1.00	71.59
ATOM	3664	C	ARG	477	83.546	3.414	4.484	1.00	46.25
ATOM ATOM	3665	0	ARG	477	82.957	2.481	5.013	1.00	46.36
ATOM	3666 3668	N	LEU	478	82.913	4.372	3.815	1.00	42.23
ATOM	3669	CA CB	LEU	478	81.464	4.418	3.743	1.00	38.89
ATOM	3670	CG	LEU LEU	478 478	80.938	5.537	4.657	1.00	37.17
ATOM	3671	CD1	LEU	478	79.418	5.733	4.678	1.00	34.13
ATOM	3672	CD2	LEU	478	78.777	4.723	5.609	1.00	32.24
ATOM	3673	C	LEU	478	79.074 81.059	7.133	5.101	1.00	33.15
ATOM	3674	0	LEU	478	81.515	4.697 5.671	2.303 1.711	1.00	38.34
ATOM	3675	N	VAL	479	80.208	3.850	1.711	1.00	40.88 37.34
ATOM	3677	CA	VAL	479	79.763	4.042	0.364	1.00	37.61
ATOM	3678	СВ	VAL	479	80.105	2.829	-0.563	1.00	36.57
ATOM	3679	CG1	VAL	479	79.647	3.105	-1.994	1.00	31.59
ATOM	3680	CG2	VAL	479	81.608	2.567	-0.561	1.00	36.11
ATOM	3681	C	VAL	479	78.267	4.277	0.375	1.00	39.24
ATOM	3682	0	VAL	479	77.484	3.358	0.619	1.00	39.16
ATOM	3683	N	LEU	480	77.894	5.528	0.142	1.00	41.32
MOTA	3685	CA	LEU	480	76.505	5.960	0.123	1.00	41.60,
MOTA	3686	СВ	LEU	480	76.446	7.480	-0.008	1.00	41.31
MOTA	3687	CG	LEU	480	77.129	8.257	1.118	1.00	39.82
ATOM	3688	CD1	LEU	480	76.985	9.737	0.856	1.00	37.96
ATOM	3689	CD2	LEU	480	76.512	7.887	2.458	1.00	37.70
MOTA	3690	C	LEU	480	75.733	5.312	-1.015	1.00	41.85
MOTA	3691	o	LEU	480	76.235	5.224	-2.131	1.00	45.02
MOTA	3692	N	GLY	481	74.501	4.897	-0.727	1.00	40.86

MOTA GLY 481 73.673 4.247 3694 CA -1.727 1.00 40.21 **ATOM** 3695 C, GLY 481 72.270 4.806 -1.873 1.00 39.78 MOTA 3696 О GLY 481 72.058 6.015 -1.810 1.00 41.68 ATOM Ν 482 3697 LYS 71.306 3.914 -2.063 1.00 39.98 69.910 MOTA 3699 CA LYS 482 4.297 -2.249 1.00 42.13 MOTA 3700 CB LYS 482 69.061 3.056 -2.566 1.00 42.73 MOTA 3701 C LYS 482 69.284 5.050 -1.084 1.00 43.13 ATOM 3702 0 LYS 482 69.373 4.625 0.060 1.00 44.49 ATOM 3703 N PRO 483 68.676 6.204 -1.358 1.00 43.22 MOTA 3704 CD PRO 483 68.708 6.969 -2.613 1.00 44.40 MOTA 3705 CA PRO 483 68.044 6.973 -0.290 1.00 45.44 ATOM 3706 PRO 483 CB 67.701 8.295 -0.980 1.00 45.01 **ATOM** 3707 CG PRO 483 67.573 7.923 -2.414 1.00 43.95 **ATOM** 3708 C PRO 483 66.801 6.261 0.232 1.00 47.67 **ATOM** 3709 0 PRO 483 66.012 5.725 -0.547 1.00 46.76 MOTA 3710 N LEU 484 66.650 6.242 1.552 1.00 49.68 MOTA 3712 CA LEU 484 65.514 5.598 2.196 1.00 54.51 MOTA 3713 CB LEU 484 65.935 5.026 3.555 1.00 52.70 MOTA 3714 CG LEU 484 67.132 4.066 3.530 1.00 51.83 **ATOM** 3715 CD1 LEU 484 67.620 3.766 4.933 1.00 50.19 **ATOM** 3716 CD2 LEU 484 66.755 2.788 2.825 1.00 52.22 ATOM 3717 LEU С 484 64.317 6.554 2.357 1.00 58.82 ATOM 3718 LEU O 484 63.158 6.138 2.244 1.00 60.07 MOTA 3719 GLY N 485 64.599 7.831 2.609 1.00 61.91 ATOM 3721 CA GLY 485 63.538 8.810 2.778 1.00 65.89 MOTA 3722 C GLY 485 64.057 10.16.7 3.227 1..00 69.46 ATOM 3723 O GLY 485 65.230 10.301 1.00 3.597 70.65 ATOM 3724 GLU N 486 63.178 11.165 3.241 1.00 70.72 MOTA 3726 CA GLU 486 63.563 12.521 3.624 1.00 71.32 ATOM 3727 CB GLU 486 64.015 13.298 2.389 1.00 73.69 ATOM 3728 C GLU 486 62.435 13.269 4.312 1.00 70.93 MOTA 3729 0 GLU 486 61.281 12.846 4.275 1.00 71.58 **ATOM** 3730 N GLY 487 62.781 14.404 4.909 1.00 70.10 MOTA 3732 CA GLY 487 61.798 15.211 5.603 1.00 68.11 MOTA 3733 C GLY 487 62.218 16.669 5.598 1.00 67.97 ATOM 3734 0 GLY 487 62.938 17.109 4.696 1.00 67.68 MOTA 3735 ALA 488 61.780 17.409 Ν 6.615 1 00 67.26 6.737 ATOM 3737 CA ALA 488 62.106 18.826 1.00 66.90 ATOM 3738 CB ALA 488 7.909 1.00 61.362 19.428 68.72 ATOM 3739 C ALA 488 63.607 19.004 6.921 1.00 67.08 MOTA 3740 488 0 ALA 64.124 18.867 8.037 1.00 65.97 MOTA 3741 N PHE 489 64.297 19.248 5.806 1.00 66.76 ATOM 3743 CA PHE 489 65.754 19.439 5.773 1.00 65.91 ATOM 3744 CB PHE 489 20.794 66.134 6.379 1.00 66.45 MOTA 3745 PHE 489 66.563 18.288 6.414 1.00 C 63.92 MOTA 3746 0 PHE 489 67.622 18.503 7.031 1.00 63.16 MOTA 3747 N GLY 490 66.067 17.069 6.209 1.00 59.03 ATOM 3749 CA GLY 490 66.710 15.878 6.720 1.00 51.12 ATOM 3750 C GLY490 14.823 1.00 66.619 5.638 48.59 **ATOM** 3751 0 GLY 490 65.608 14.736 4.938 1.00 45.25 MOTA 3752 GLN 491 67.659 14.003 5.525 N 1.00 48.77 MOTA 3754 CA GLN 491 67.732 12.951 4.519 1.00 47.40 MOTA 3755 CB GLN 491 68.529 13.474 3.319 1.00 49.92 MOTA 3756 CG GLN 491 68.653 12.514 2.155 1.00 56.31

ATOM	3757	CD	GLN	491	69.604	13.020	1.088	1.00	58.79
ATOM	3758	OE1	GLN	491	70.043	14.171	1.130	1.00	59.63
MOTA	3759	NE2	GLN	491	69.929	12.161	0.122	1.00	59.05
MOTA	3762	С	GLN	491	68.407	11.693	5.086	1.00	44.46
MOTA	3763	0	GLN	491	69.396	11.782	5.806	1.00	44.15
ATOM	3764	N	VAL	492	67.867	10.527	4.752	1.00	42.55
MOTA	3766	CA	VAL	492	68.416	9.247	5.205	1.00	39.22
ATOM	3767	CB	VAL	492	67.375	8.458	6.042	1.00	39.40
MOTA	3768	CG1	VAL	492	67.947	7.127	6.524	1.00	40.17
MOTA	3769	CG2	VAL	492	66.922	9.267	7.210	1.00	36.12
ATOM	3770	С	VAL	492	68.746	8.396	3.975	1.00	37.57
MOTA	3771	0	VAL	492	67.888	8.178	3.115	1.00	35.70
MOTA	3772	N	VAL	493	69.990	7.961	3.845	1.00	36.27
ATOM	3774	CA	VAL	493	70.333	7.127	2.711	1.00	37.61
MOTA	3775	CB	VAL	493	71.237	7.863	1.643	1.00	37.45
MOTA	3776	CG1	VAL	493	70.836	9.319	1.524	1.00	38.29
ATOM	3777	CG2	VAL	493	72.717	7.713	1.943	1.00	36.53
ATOM	3778	С	VAL	493	70.952	5.806	3.156	1.00	37.54
ATOM	3779	0	VAL	493	71.542	5.711	4.233	1.00	37.32
ATOM	3780	N	LEU	494	70.691	4.763	2.380	1.00	37.67
ATOM	3782	CA	LEU	494	71.236	3.450	2.656	1.00	38.41
MOTA	3783	CB	LEU	494	70.482	2.387	1.851	1.00	39.16
MOTA	3784	CG	LEU	494	70.834	0.908	2.021	1.00	36.43
ATOM	3785	CD1	LEU	494	70.809	0.508	3.479	1.00	34.69
ATOM	3786	CD2	LEU	494	69.840	0.086	1.229	1.00	37.48
MOTA	3787	С	LEU	494	72.683	3.541	2.202	1.00	39.30
ATOM	3788	0	LEU	494	72.976	4.201	1.207	1.00	39.21
MOTA	3789	N	ALA	495	73.584	2.922	2.954	1.00	40.08
ATOM	3791	CA	ALA	495	74.996	2.954	2.619	1.00	41.70
ATOM	3792	CB	ALA	495	75.654	4.162	3.283	1.00	41.63
MOTA	3793	С	ALA	495	75.670	1.669	3.080	1.00	43.92
MOTA	3794	0	ALA	495	75.033	0.818	3.711	1.00	45.20
MOTA	3795	N	GLU	496	76.946	1.515	2.731	1.00	44.21
MOTA	3797	CA	GLU	496	77.712	0.347	3.137	1.00	43.44
MOTA.	3798	CB	GLU	496	78.046	-0.538	1.943	1.00	45.87
MOTA	3799	CG	GLU	496	76.816	-1.142	1.301	1.00	53.11
ATOM	3800	CD	GLU	496	77.145	-2.262	0.339	1.00	56.68
MOTA	3801	OE1	GLU	496	76.473	-3.316	0.410	1.00	61.87
MOTA	3802	OE2	GLU	496	78.068	-2.091	-0.482	1.00	58.18
ATOM	3803	С	GLU	496	78.973	0.773	3.860	1.00	40.97
MOTA	3804	0	GLU	496	79.835	1.437	3.302	1.00	40.91
ATOM	3805	N	ALA	497	79.036	0.439	5.136	1.00	42.07
MOTA	3807	CA	ALA	497	80.173	0.786	5.959	1.00	43.69
MOTA	3808	CB	ALA	497	79.709	1.104	7.366	1.00	40.90
ATOM	3809	С	ALA	497	81.160	-0.372	5.962	1.00	46.16
MOTA	3810	0	ALA	497	80.764	-1.525	5.814	1.00	46.90
MOTA	3811	N	ILE	498	82.446	-0.059	6.090	1.00	48.78
MOTA	3813	CA	ILE	498	83.494	-1.068	6.114	1.00	49.59
ATOM	3814	СВ	ILE	498	84.395	-0.993	4.858	1.00	49.46
MOTA	3815	CG2	ILE	498	85.524	-2.006	4.954	1.00	51.16
MOTA	3816	CG1	ILE	498	83.577	-1.244	3.591	1.00	48.96
ATOM	3817	CD1	ILE	498	82.924	0.009	2.998	1.00	52.50
ATOM	3818	С	ILE	498	84.352	-0.877	7.355	1.00	51.33
ATOM	3819	0	ILE	498	84.818	0.230	7.641	1.00	50.42
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ATOM	3820	N	GLY	499	84.506	-1.952	8.119	1.00	53.87
ATOM	3822	CA	GLY	499	85.314	-1.909	9.324	1.00	58.16
ATOM	3823	С	GLY	499	84.759	-1.094	10.483	1.00	62.44
ATOM	3824	0	GLY	499	85.510	-0.400	11.175	1.00	65.17
ATOM	3825	N	LEU	500	83.454	-1.187	10.720	1.00	62.92
MOTA	3827	CA	LEU	500	82.839	-0.453	11.822	1.00	61.93
MOTA	3828	CB	LEU	500	81.339	-0.752	11.888	1.00	58.77
ATOM	3829	CG	LEU	500	80.501	-0.207	10.736	1.00	56.68
ATOM	3830	CD1	LEU	500	79.047	-0.547	10.964	1.00	55.05
ATOM	3831	CD2	LEU	500	80.682	1.298	10.635	1.00	56.30
ATOM	3832	C	LEU	500	83.501	-0.820	13.149	1.00	63.28
ATOM	3833	0	LEU	500	83.623	-2.002	13.487	1.00	64.91
MOTA	3834	N	PRO	505	87.387	-6.451	10.091	1.00	82.92
MOTA	3835	CD	PRO	505	88.522	-6. <b>96</b> 6	10.874	1.00	83.74
ATOM	3836	CA	PRO	505	87.618	-5.052	9.705	1.00	80.73
ATOM	3837	CB	PRO	505	89.027	-4.770	10.247	1.00	81.95
ATOM	3838	CG	PRO	505	89.655	-6.133	10.342	1.00	83.54
ATOM	3839	C	PRO	505	87.514	-4.794	8.205	1.00	77.60
ATOM	3640	0	PRO	505	87.445	-3.651	7.761	1.00	77.24
ATOM	3841	N	ASN	506	87.488	-5.863	7.424	1.00	75.24
ATOM	3843	CA	ASN	506	87.380	-5.727	5.981	1.00	72.92
ATOM	3844	CB	ASN	506	88.435	-6.589	5.283	1.00	73.87
ATOM ATOM	3845	C.	ASN	506	85.978	-6.122	5.529	1.00	70.43
ATOM	3846 3847	0	ASN	506	85.719	-6.281	4.340	1.00	70.01
ATOM		N	ARG	507	85.075		6.491	1.00	68.31
ATOM	3849 3850	CA CB	ARG ARG	507	83 697	-6.647	6.200	1.00	65.59
ATOM	3851	CB		507	83.112	-7.429	7.378	1.00	66.34
ATOM	3852	0	ARG	507	82.846	-5.413	5.941	1.00	62.97
ATOM	3853	N	ARG	507	83.191	-4.313	6.375	1.00	63.16
ATOM	3855	CA	VAL VAL	508 508	81.740	-5.599	5.231	1.00	60.02
ATOM	3856	CB	VAL	508	80.840 80.532	-4.495	4.947	1.00	58.59
ATOM	3857	CG1	VAL	508	81.813	··4.357	3.439	1.00	58.40
ATOM	3858	CG2	VAL	508	79.751	-4.196 -5.553	2.658 2.938	1.00	61.14
ATOM	3859	C	VAL	508	79.537	-4.682	5.707	1.00	61.01
ATOM	3860	0	VAL	508	79.031	-5.803	5.836	1.00 1.00	57.24
ATOM	3861	N	THR	509	79.020	-3.579	6.237	1.00	58.42
ATOM	3863	CA	THR	509	77.769	-3.572	6.973	1.00	54.22 48.99
ATOM	3864	CB	THR	509	77.971	-3.100	8.428	1.00	49.59
ATOM	3865	OG1	THR	509	78.932	-3.935	9.082	1.00	51.71
ATOM	3867	CG2	THR	509	76.665	-3.166	9.198	1.00	50.69
MOTA	3868	C	THR	509	76.837	-2.606	6.253	1.00	46.51
ATOM	3869	0	THR	509	77.231	-1.503	5.886	1.00	44.91
ATOM	3870	N	LYS	510	75.628	-3.059	5.966	1.00	45.65
ATOM	3872	CA	LYS	510	74.658	-2.208	5.314	1.00	43.61
ATOM	3873	СВ	LYS	510	73.598	-3.058	4.632	1.00	45.46
MOTA	3874	CG	LYS	510	72.845	-2.306	3.568	1.00	54.00
ATOM	3875	CD	LYS	510	73.022	-2.912	2.183	1.00	58.74
ATOM	3876	CE	LYS	510	72.194	-4.184	2.007	1.00	59.63
ATOM	3877	NZ	LYS	510	72.711	-5.323	2.815	1.00	61.62
ATOM	3881	C	LYS	510	74.065	-1.359	6.450	1.00	42.05
ATOM	3882	0	LYS	510	73.566	-1.898	7 439	1.00	41.29
MOTA	3883	N	VAL	511	74.185	-0.038	6.333	1.00	40.14
ATOM	3885	CA	VAL	511	73.719	0.894	7.359	1.00	35.38
			-	-	,	054		2.00	55.50

ATOM 3886 CB VAL 511 74.932 1.554 8.074 1.00 33.16 ATOM 3887 CG1 VAL 511 75.761 0.501 8.795 1.00 29.24 MOTA 3888 CG2 VAL 511 75.804 2.295 7.054 1.00 30.37 **ATOM** 3889 VAL С 511 72.856 2.005 6.776 1.00 33.90 **ATOM** 3890 0 VAL 511 72.722 2.110 5.558 1.00 32.53 **ATOM** 3891 N ALA 512 72.261 7.655 2.813 1.00 31.97 **ATOM** 3893 CA ALA 512 71.434 3.956 7.248 1.00 31.10 MOTA 3894 CB ALA 512 70.088 3.945 7.952 1.00 27.38 ATOM 3895 C ALA 512 72.225 5.186 7.660 1.00 30.49 MOTA 3896 0 ALA 512 72.775 5.235 8.766 1.00 30.10 MOTA 3897 N VAL 513 72.312 6.162 6.765 1.00 30.50 ATOM 3899 CA VAL 513 73.064 7.382 7.041 1.00 29.68 MOTA 3900 VAL CB 513 74.204 7.593 6.015 1.00 28.89 3901 **ATOM** CG1 VAL 513 74.966 8.856 6.334 1.00 26.30 MOTA 3902 CG2 VAL 513 75.134 6.389 5.987 1.00 26.66 MOTA 3903 C VAL 513 8.607 72.171 7.012 1.00 28.50 **ATOM** 3904 VAL 0 513 71.536 8.893 5.994 1.00 26.27 ATOM 3905 N LYS 514 72.091 9.282 8.154 1.00 29.18 ATOM 3907 CA LYS 514 71.307 10.508 8.295 1.00 31.52 ATOM 3908 LYS CB 514 70.797 10.659 9.728 1.00 33.52 MOTA 3909 CG LYS 514 69.890 9.540 10.198 1.00 35.67 MOTA 3910 CD LYS 514 69.439 9.831 11.618 1.00 44.89 MOTA 3911 LYS CE 514 68.313 8.909 12.060 1.00 51.12 MOTA 3912 NZ LYS 514 67.029 9.137 11.307 1.00 57.11 ATOM 3916 C LYS 514 72.233 11.681 7.956 1.00 30.75 MOTA 3917 0 LYS 514 73.390 11.698 8.379 1.00 30.08 MOTA 3918 N MET 51.5 71.724 12.651 7.201 1.00 29.45 MOTA 3920 CA MET 515 72.511 13.814 6.786 1.00 28.74 MOTA 3921 CBMET 515 73.342 13.466 5.552 1.00 27.72 MOTA 3922 CG MET 515 72.487 13.034 4.378 1.00 31.56 MOTA 3923 SD MET 515 73.442 12.549 2.945 1.90 34.98 MOTA 3924 CE MET 515 73.730 10.878 3.330 1.00 31.23 MOTA 3925 C MET 515 71.585 14.966 6.444 1.00 27.75 MOTA 3926 0 MET 515 70.369 14.794 6.359 1.00 29.07 ATOM 3927 N LEU 516 72.152 16.145 6.247 1.00 28.33 ATOM 3929 CA LEU 516 71.348 17.313 5.912 1.00 31.16 ATOM 3930 CB LEU 516 72.052 18.605 6.339 1.00 28.70 **ATOM** 3931 CG LEU 18.866 516 72.312 7.826 1.00 28.33 **ATOM** 3932 CD1 LEU 516 73.098 20.156 7.949 1.00 28.45 **ATOM** 3933 CD2 LEU 516 71.020 18.959 8.604 1.00 21.64 MOTA 3934 С LEU 516 71.069 17.378 4.421 1.00 33.22 **ATOM** 3935 0 LEU 516 71.762 16.760 3.619 1.00 35.00 **ATOM** 3936 N LYS 517 70.022 18.100 4.061 1.00 34.69 ATOM 3938 CA LYS 517 69.696 18.286 2.665 1.00 34.20 MOTA 3939 CB LYS 517 68.194 18.475 2.496 1.00 37.45 ATOM 3940 CG LYS 517 67.403 2.950 17.264 1.00 43.71 MOTA 3941 CD LYS 517 66.157 17.072 2.126 1.00 51.25 ATOM 3942 CE LYS 517 65.123 18.135 2.419 1.00 58.56 MOTA 3943 NZ LYS 517 64.010 18.049 1.438 1.00 63.12 MOTA 3947 С LYS 517 70.482 19.533 2.259 1.00 33.81 MOTA 3948 0 LYS 517 70.991 20.244 3.130 1.00 33.17 MOTA 3949 N SER 518 70.603 19.788 0.959 1.00 33.42 MOTA 3951 CA SER 518 71.369 20.938 0.472 1.00 33.33 MOTA 3952 CB SER 518 71.550 20.842 -1.042 1.00 33.23

MOTA	3953	OG	SER	518	70.306	20.624	-1.678	1.00	38.84
ATOM	3955	C	SER	518	70.794	22.298	0.846	1.00	33.23
ATOM	3956	0	SER	518	71.509	23.305	0.865	1.00	34.14
MOTA	3957	N	ASP	519	69.510	22.313	1.178	1.00	32.77
MOTA	3959	CA	ASP	519	68.825	23.541	1.570	1.00	33.26
MOTA	3960	CB	ASP	519	67.401	23.563	0.995	1.00	35.10
ATOM	3961	CG	ASP	519	66.484	22.503	1.617	1.00	38.98
ATOM	3962	OD1	ASP	519	66. <del>9</del> 58	21.430	2.042	1.00	37.30
ATOM	3963	OD2	ASP	519	65.261	22.754	1.674	1.00	43.65
ATOM	3964	С	ASP	519	68.793	23.747	3.091	1.00	33.05
ATOM	3965	0	ASP	519	68.114	24.648	3.580	1.00	
ATOM	3966	N	ALA	520	69.538	22.931	3.833	1.00	35.19
ATOM	3968	CA	ALA	520	69.570	23.032	5.293	1.00	31.38
ATOM	3969	CB	ALA	520	70.264	21.830	5.870		29.47
ATOM	3970	C	ALA	520	70.229	24.301	5.812	1.00	29.74
ATOM	3971	0	ALA	520	71.004	24.952	5.106	1.00	29.83
ATOM	3972	N	THR	521	69.938	24.616	7.071	1.00 1.00	30.23
ATOM	3974	CA	THR	521	70.487	25.793	7.742		31.57
ATOM	3975	СВ	THR	521	69.361	26.736		1.00	34.56
ATOM	3976	OG1	THR	521	68.670	26.082	9.302	1.00	38.37
ATOM	3978	CG2	THR	521	68.357	27.117	9.376	1.00	41.75
ATOM	3979	C	THR	521	71.353	25.363	7.209	1.00	38.30
ATOM	3980	ō	THR	521	71.320	24.207	8.916	1.00	33.22
ATOM	3981	N	GLU	522	72.092	26.310	9.327	1.00	32.31
ATOM	3983	CA	GLU	522	72.951	26.042	9.479	1.00	34.43
ATOM	3984	СВ	GLU	522	73.634	27.340	10.619	1.00	39.53
ATOM	3985	CG	GLU	522	74.398	27.340	11.068	1.00	46.35
ATOM	3986	CD	GLU	522	75.772	26.603	12.402	1.00	58.03
ATOM	3987	OE1	GLU	522	76.800	27.321	12.301	1.00	63.14
ATOM	3988	QE2	GLU	522	75.824	25.359	12.404	1.00	61.75
ATOM	3989	C	GLU	522	72.130	25.428	12.158	1.00	66.35
ATOM	3990	С	GLU	522	72.642	24.622	11.765	1.00	38.40
MOTA	3991	N	LYS	523	70.853	25.792	12.543 11.849	1.00	37.92
MOTA	3993	CA	LYS	523	69.995	25.752	12.893	1.00	36.43
ATOM	3994	CB	LYS	523	68.703	26.065	13.008	1.00	36.83
MOTA	3995	CG	LYS	523	67.793	25.636		1.00	40.88
ATOM	3996	CD	LYS	523	66.584	24.898	14.152 13.607	1.00	44.55
MOTA	3997	CE	LYS	523	65.629	24.483	14.708	1.00	52.68
ATOM	3998	NZ	LYS	523	64.537	23.646	14.123	1.00	56.04
ATOM	4002	С	LYS	523	69.689	23.804		1.00	58.13
MOTA	4003	0	LYS	523	69.645	22.985	12.601 13.513	1.00	35.27
ATOM	4004	N	ASP	524	69.496	23.473	11.326	1.00	36.58
ATOM	4006	CA	ASP	524	69.235	22.089		1.00	32.27
ATOM	4007	CB	ASP	524	68.952	21.953	10.963	1.00	27.18
ATOM	4008	CG	ASP	524	67.635	22.555	9.480	1.00	26.32
ATOM	4009	OD1	ASP	524	66.662		9.089	1.00	25.22
ATOM	4010	OD2	ASP	524	67.568	22.394	9.848	1.00	31.78
ATOM	4011	C	ASP	524	70.445	23.190	8.028	1.00	24.00
ATOM	4012	0	ASP	524		21.268	11.342	1.00	26.83
ATOM	4013	N	LEU	525	70.312 71.633	20.165	11.851	1.00	28.65
ATOM	4015	CA	LEU	525		21.827	11.129	1.00	28.69
ATOM	4016	CB	LEU	525	72.872	21.148	11.473	1.00	26.96
ATOM	4017	CG	LEU	525	74.077	21.981	11.049	1.00	22.80
ATOM	4018	CD1	LEU		75.445	21.355	11.341	1.00	22.32
,	1010	CDI	ne O	525	75.522	19.883	10.858	1.00	18.89

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ATOM	4019	CD2	LEU	525	76.504	22.212	10.704	1.00	17.44
ATOM	4020	С	LEU	525	72.886	20.926	12.980	1.00	28.00
ATOM	4021	0	LEU	525	73.160	19.816	13.462	1.00	28.82
ATOM	4022	N	SER	526	72.567	21.992	13.707	1.00	27.98
ATOM	4024	CA	SER	526	72.496	21.994	15.168	1.00	30.78
ATOM	4025	CB	SER	526	71.939	23.345	15.627	1.00	33.18
ATOM	4026	OG	SER	526	71.624	23.347	17.009	1.00	42.73
ATOM	4028	С	SER	526	71.599	20.865	15.704	1.00	30.56
MOTA	4029	0	SER	526	71.906	20.206	16.716	1.00	31.92
MOTA	4030	N	ASP	527	70.484	20.665	15.018	1.00	28.19
MOTA	4032	CA	ASP	527	69.516	19.651	15.366	1.00	27.41
ATOM	4033	CB	ASP	527	68.207	19.932	14.632	1.00	27.63
ATOM	4034	CG	ASP	527	67.492	21.172	15.149	1.00	27.37
MOTA	4035	OD1	ASP	527	67.870	21.728	16.211	1.00	26.70
MOTA	4036	OD2	ASP	527	66.525	21.579	14.487	1.00	33.80
ATOM	4037	C	ASP	527	70.007	18.241	15.063	1.00	27.36
MOTA	4038	О	ASP	527	69.722	17.309	15.816	1.00	30.13
MOTA	4039	N.	LEU	528	70.716	18.077	13.952	1.00	25.76
ATOM	4041	CA	LEU	528	71.245	16.765	13.588	1.00	25.29
ATOM	4042	CB	LEU	528	. =	16.771	12.143	1.00	23.65
ATOM	4043	CG	LEU	528	72.283	15.432	11.574	1.00	25.86
MOTA	4044	CD1	LEU	528	71.234	14.341	11.770	1.00	23.35
MOTA	4045	CD2	LEU	528	72.652	15.566	10.102	1.00	17.46
MOTA	4046	C	LEU	528	72.351	16.368	14.578	1.00	25.66
MOTA	4047	С	LEU	528	72.418	15.210	15.015	1.00	24.02
MOTA	4048	N	ILE	529	73.200	17.338	14.934	1.00	26.36
ATOM	4050	CA	ILE	529	74.304	17.130	15.886	1.00	26.17
MOTA	4051	CB	ILE	529	75.192	18.381	16.003	1.00	22.72
ATOM	4052	CG2	ILE	529	76.250	18.180	17.057	1.00	21.32
ATOM	4053	CG1	ILE	529	75.876	18.666	14.685	1.00	20.71
ATOM	4054	CD1	ILE	529	76.621	19.965	14.675	1.00	25.60
MOTA	4055	C	ILE	529	73.756	16.835	17.283	1.00	29.87
MOTA	4056	<b>O</b>	ILE	529	74.253	15.948	17.977	1.00	32.20
MOTA	4057	N	SER	530	72.741	17.591	17.693	1.00	28.63
ATOM	4059	CA	SER	530	72.143	17.381	18.991	1.00	32.21
ATOM	4060	CB	SER	530	71.031	18.399	19.231	1.00	37.45
ATOM	4061	OG	SER	530	70.065	18.342	18.195	1.00	49.52
ATOM	4063	C	SER	530	71.598	15.956	19.075	1.00	30.96
ATOM	4064	0	SER	530	71.728	15.301	20.105	1.00	33.05
MOTA	4065	N	GLU	531	70.996	15.476	17.996	1.00	29.13
ATOM	4067	CA	GLU	531	70.468	14.117	17.987	1.00	29.84
ATOM	4068	CB	GLU	531	69.672	13.847	16.709	1.00	30.29
ATOM	4069	CG	GLU	531	69.093	12.445	16.666	1.00	27.39
ATOM	4070	CD	GLU	531	68.521	12.074	15.331	1.00	31.34
ATOM	4071	OE1	GLU	531	67.929	10.981	15.228	1.00	35.90
ATOM	4072	OE2	GLU	531	68.660	12.860	14.376	1.00	38.37
ATOM	4073	C	GLU	531	71.600	13.081	18.109	1.00	28.48
ATOM	4074	0	GLU	531	71.468	12.094	18.822	1.00	28.17
ATOM	4075	N	MET	532	72.682	13.281	17.364	1.00	28.12
MOTA	4077	CA	MET	532	73.832	12.376	17.409	1.00	27.64
ATOM	4078	CB	MET	532	74.953	12.899	16.499	1.00	26.47
ATOM	4079	CG	MET	532	76.267	12.125	16.601	1.00	22.25
ATOM	4080	SD	MET	532	77.406	12.610	15.286	1.00	30.32
ATOM	4081	CE	MET	532	77.613	14.366	15.661	1.00	20.92

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ATO		_	ME'	r 532	74.339	12.32	8 18.83	2 1.00	27.87	,
ATO			ME		74.640	11.26				
ATO			GL		74.439	13.49				
ATO	•				74.906	13.594				
ATO!					75.071	15.064				
ATO		_			76.216	15.745				
ATO					77.564	15.070		•		
ATOM	_				78.001	14.969				
ATON					78.202	14.643				
ATOM			GLU		73.981	12.850				
ATOM		-	GLU		74.455	12.093			29.73	
ATOM			MET	534	72.670	13.014			29.70	
ATOM			MET	534	71.692	12.346			27.97	
ATOM		-	MET	534	70.258	12.751			28.95	
ATOM			MET	534	69.311	12.594		0.50	29.62	רידעם
ATOM		_	MET	534	67.538	12.682	22.961	0.50	29.87	
ATOM			MET	534	67.269	14.452	22.795	0.50	31.07	PRT1
ATOM			MET	534	71.855	10.821	22.362	1.00	28.36	1111
ATOM			MET	534	71.833	10.143	23.386	1.00	27.02	
ATOM			MET	535	72.048	10.297	21.151	1.00	26.96	
ATOM			MET	535	72.239	8.861	20.947	1.00	26.63	
ATOM	4107	CB	MET	535	72.347	8.521	19.456	1.00	24.67	
ATOM	4108	CG SD	MET	535	71.089	8.778	18.659	1.00	23.15	
ATOM	4109	CE	MET	535	71.160	8.062	17.011	1.00	24.57	
ATOM	4110	C	MET	535	71.251	9.486	16.023	1.00	24.79	
ATOM	4111	0	MET MET	535	73.498	8.390	21.669	1.00	27.66	
ATOM	4112	N		535	73.564	7.259	22.164	1.00	28.83	
ATOM	4114	CA	LYS LYS	536 536	74.515	9.246	21.698	1.00	29.13	
ATOM	4115	CB	LYS	536	75.757	8.918	22.392	1.00	30.50	
ATOM	4116	CG	LYS	536 536	76.812	9.985	22.131	1.00	29.15	
ATOM	4117	CD	LYS	536	77.499	9.883	20.802	1.00	27.71	
ATOM	4118	CE	LYS	536	78.377 79.085	11.100	20.615	1.00	28.12	
ATOM	4119	NZ	LYS	536	79.688	11.096	19.279	1.00	26.89	
ATOM	4123	С	LYS	536	75.480	12.436	19.077	1.00	27.54	
ATOM	4124	0	LYS	536	75.921	8.836	23.892	1.00	31.92	
ATOM	4125	N	MET	537	74.742	7.908	24.559	1.00	31.19	
MOTA	4127	CA	MET	537	74.384	9.814	24.409	1.00	34.02	
ATOM	4128	CB	MET	537	73.648	9.881 11.197	25.822	1.00	36.35	
ATOM	4129	CG	MET	537	73.096	11.197	26.083	1.00	43.33	
ATOM	4130	SD	MET	537	71.426	10.674	27.507	1.00	54.60	
ATOM	4131	CE	MET	537	71 684	9.813	27.856	1.00	67.38	
ATOM	4132	C	MET	537	73.507	8.705	29.440	1.00	62.03	
ATOM	4133	0	MET	537	73.744	8.069	26.253 27.275	1.00	34.53	
MOTA	4134	N	ILE	538	72.496	8.425		1.00	36.76	
ATOM	4136	CA	ILE	538	71.568	7.367	25.454 25.757	1.00	32.24	
MOTA	4137	CB	ILE	538	70.396	7.384		1.00	29.88	
ATOM	4138	CG2	ILE	538	69.582	6.096	24.757 24.842	1.00	26.98	
ATOM	4139	CG1	ILE	538	69.527	8.614		1.00	27.93	
MOTA	4140	CD1	ILE	538	68.399	8.787	25.036 24.058	1.00	22.58	
ATOM	4141	C		538	72.236	6.006	25.804		24.58	
MOTA	4142	0		538	71.983	5.227	26.713		31.83	
ATOM	4143	N		<b>5</b> 39	73.102	5.718	24.848		36.32	
MOTA	4145	CA		539	73.744	4.422	24.850		32.45	
					_		_2.050	1.00	32.13	

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,	MOTA	4146	С	GLY	539	72.974	3.380	24.056	1.00	33.83
7	MOTA	4147	0	GLY	539	71.876	3.654	23.530	1.00	33.75
Į	MOTA	4148	N	LYS	540	73.539	2.173	24.010	1.00	33.36
7	MOTA	4150	CA	LYS	540	72.980	1.054	23.256	1.00	37.04
7	MOTA	4151	CB	LYS	540	74.110	0.181	22.709	1.00	39.21
I	MOTA	4152	CG	LYS	540	74.865	0.893	21.623	1.00	48.72
Į	MOTA	4153	CD	LYS	540	75.818	0.009	20.850	1.00	56.84
7	MOTA	4154	CE	LYS	540	76.225	0.693	19.516	1.00	62.14
P	MOTA	4155	NZ	LYS	540	77.252	-0.102	18.805	1.00	71.02
P	MOTA	4159	С	LYS	540	71.938	0.162	23.901	1.00	36.51
7	MOTA	4160	0	LYS	540 .	71.963	-0.096	25.113	1.00	38.52
P	MOTA	4161	N	HIS	541	71.017	-0.295	23.058	1.00	32.98
7	MOTA	4163	CA	HIS	541	69.963	-1.230	23.424	1.00	31.20
Þ	MOTA	4164	CB	HIS	541	68.779	-0.561	24.095	1.00	30.35
Α	MOTA	4165	CG	HIS	541	67.815	-1.540	24.694	1.00	32.56
₽	MOTA	4166	CD2	HIS	541	67.737	-2.058	25.941	1.00	32.45
P	MOTA	4167	ND1	HIS	541	66.795	-2.124	23.974	1.00	29.22
P	MOTA	4169	CEl	HIS	541	66.134	-2.965	24.753	1.00	31.56
A	MOTA	4170	NE2	HIS	541	66.679	-2.932	25.957	1.00	32.22
A	MOTA	4172	C	HIS	541	69.509	-1.937	22.152	1.00	32.00
A	MOTA	4173	O	HIS	541	69.409	-1.324	21.095	1.00	32.84
A	MOT	4174	N	LYS	542	69.187	-3.222	22.273	1.00	33.61
A	MOT	4176	CA	LYS	542	68.786	-4.061	21.154	1.00	31.54
A	MOTA	4177	CB	LYS	542	68.653	-5.516	21.596	1.00	33.94
	TOM	4178	CG	LYS	542	6.8 . 322	-6.451	20.437	1.00	42.34
A	MOT	4179	CD	LYS	542	68.083	-7.885	20.856	1.00	47.57
	MOT	4180	CE	LYS	542	67.634	-8.726	19.658	1.00	52.70
	MOT	4181	NZ	LYS	542	67.402	-10.146	20.023	1.00	59.51
	MOT	4185	C	LYS	542	67.495	-3.611	20.487	1.00	29.57
	MOT	4186	0	LYS	542	67.268	-3.884	19.305	1.00	27.99
	TOM	4187	N	ASN	543	66.649	-2.931	21.253	1.00	28.32
	TOM	4189	CA	ASN	543	65.378	-2.476	20.714	1.00	28.86
	MOT	4190	CB	ASN	543	64.231	-2.947	21.601	1.00	29.33
	TOM	4191	CG	ASN	543	64.247	-4.452	21.811	1.00	29.64
	TOM	4192	OD1	ASN	543	64.437	-4.926	22.930	1.00	33.86
	TOM	4193	ND2	ASN	543	64.106	-5.206	20.732	1.00	28.02
	TOM	4196	C	ASN	543	65.252	-0.983	20.378	1.00	29.69
	TOM	4197	0	ASN	543	64.159	-0.413	20.457	1.00	30.02
	TOM	4198	N	ILE	544	66.372	-0.357	20.011	1.00	27.35
	TOM	4200	CA	ILE	544	66.382	1.046	19.593	1.00	25.95
	TOM TOM	4201	CB	ILE	544	66.898	2.030	20.706	1.00	25.56
		4202	CG2	ILE	544	66.148	1.819	22.037	1.00	21.06
	MOT.	4203	CG1	ILE	544	68.406	1.901	20.902	1.00	25.61
	TOM	4204	CD1	ILE	544	68.952	2.818	21.976	1.00	25.89
	TOM	4205	C	ILE	544	67.341	1.083	18.399	1.00	25.97
	TOM	4206	0	ILE	544	68.126	0.152	18.227	1.00	25.69
	TOM	4207	N	ILE	545	67.226	2.095	17.537	1.00	27.27
	TOM	4209	CA	ILE	545	68.129	2.243	16.384	1.00	27.02
	TOM	4210	CB	ILE	545	67.541	3.194	15.307	1.00	27.30
	TOM	4211	CG2	ILE	545	68.592	3.553	14.269	1.00	26.52
	TOM	4212	CG1	ILE	545	66.309	2.570	14.638	1.00	22.63
	TOM	4213	CD1	ILE	545	66.605	1.447	13.665	1.00	17.57
	TOM	4214	C	ILE	545	69.383	2.873	16.979	1.00	28.55
A	TOM	4215	0	ILE	545	69.346	4.014	17.451	1.00	29.47

ATO			ASI	N 546	70.482	2 2.12	3 16.96	5 3 04	
ATO			ASI	V 546	71.748				
ATO			ASI	N 546	72.49			_	
ATC			ASI	V 546	71.732		_		
ATC			l Asn	J 546	71.580				
ATO			2 ASN		71.267				· ·
ATO			ASN	546	72.700				
ATO		_	ASN	546	72.679				
ATO			LEU	547	73.543				
ATO		9 CA	LEU	547	74.570				
ATO			LEU		75.043	6.076			
ATO			LEU	547	76.075	7.088			
ATO			LEU	547	75.553				22.12
ATO			LEU	547	76.415	7.815			22.10
ATON	423	4 C'	LEU	547	75.756	8.089		1.00	18.67
ATOM		5 0	LEU	547	76.284	4.039		1.00	30.70
ATOM		-	LEU	548	76.141	3.361		1.00	34.46
ATOM		CA	LEU	548	77.262	3.993		1.00	30.97
ATOM		CB	LEU	548	76.929	3.165		1.00	30.73
ATOM		CG	LEU	548	75.788	2.406	13.281	1.00	29.24
ATOM	4241	CD1	LEU	548	75.924	1.394	13.371	1.00	28.77
ATOM	4242	CD2	LEU	548	75.839	0.460	12.209	1.00	26.55
ATOM	4243	С	LEU	548	78.522	0.616	14.683	1.00	23.48
ATOM	4244	0	LEU	548	79.640	3.982	14.347	1.00	33.00
MOTA.	4245	N	GLY	549	78.351	3.500	14.558	1.00	35.92
ATOM	4247	CA	GLY	549	79.503	5.215	13.901	1.00	32.52
ATOM	4248	С	GLY	549	79.092	6.051	13.673	1.00	32.76
ATOM	4249	0	GLY	549	77.895	7.411	13.180	1.00	33.72
ATOM	4250	N	ALA	550	80.089	7.707	13.092	1.00	35.01
ATOM	4252	CA	ALA	550	79.848	8.226	12.840	1.00	33.47
MOTA	4253	CB	ALA	550		9.566	12.337	1.00	30.69
MOTA	4254	C	ALA	550	79.555	10.509	13.497	1.00	28.66
MOTA	4255	0	ALA	550	81.022	10.099	11.523	1.00	30.41
ATOM	4256	N ·	CYS	551	82.181	9.780	11.808	1.00	29.13
ATOM	4258	CA	CYS	551	80.695	10.817	10.446	1.00	30.29
ATOM	4259	CB	CYS	551	81.675	11.490	9.584	1.00	28.44
MOTA	4260	SG	CYS	551	81.432	11.214	8.096	1.00	27.25
ATOM	4261	С	CYS	551	81.639	9.508	7.566	1.00	28.89
MOTA	4262	0	CYS	551	81.337	12.950	9.883	1.00	27.07
ATOM	4263	N		552	80.293	13.441	9.467		29.86
ATOM	4265	CA	THR	552	82.184	13.616	10.658	1.00	25.10
ATOM	4266	CB		552 552	81.952	14.997	11.047		24.37
ATOM	4267			552 552	81.959	15.091	12.569		27.67
ATOM	4269			552 552	83.271	14.760	13.052		26.11
ATOM	4270				80.951	14.120			30.41
ATOM	4271			552 552	83.003	15.980	10.557		24.51
ATOM	4272			552 552	82.804	17.194			21.56
ATOM	4274			553	84.151	15.441			27.13
ATOM	4275			553	85.284	16.243			26.64
ATOM	4276			553	86.592	15.679			25.24
ATOM	4277			553	86.641	15.561		_	22.38
ATOM	4278			553	86.464	16.897			24.04
ATOM	4279			553	87.267	17.815		_	31.50
ATOM				553	85.403				
	4404	٠ (	ع الأماد	53	85.384	16.276			
ATOM \$\$\$(D)55	4282	С (	GLN S	553	85.384				81.59

ATOM	4283	0	GLN	553	85.069	15.293	7.537	1.00	30.20
ATOM	4284	N	ASP	554	85.794	17.430	7.695	1.00	28.08
ATOM	4286	CA	ASP	554	86.000	17.652	6.263	1.00	30.14
ATOM	4287	CB	ASP	554	87.330	17.034	5.833	1.00	29.82
MOTA	4288	CG	ASP	554	88.451	17.470	6.707	1.00	31.79
ATOM	4289	OD1	ASP	554	88.699	18.666	6.767	1.00	36.45
MOTA	4290	OD2	ASP	554	89.066	16.623	7.364	1.00	33.06
ATOM	4291	C	ASP	554	84.895	17.217	5.317	1.00	29.52
ATOM	4292	0	ASP	554	85.128	16.411	4.424	1.00	33.67
ATOM	4293	N	GLY	555	83.709	17.793	5.488	1.00	29.02
MOTA	4295	CA	GLY	555	82.586	17.476	4.621	1.00	26.05
ATOM	4296	C	GLY	555	81.286	17.447	5.405	1.00	23.80
ATOM	4297	0	GLY	555	81.269	17.751	6.597	1.00	24.09
MOTA	4298	N	PRO	556	80.175	17.117	4.740	1.00	23.29
ATOM	4299	CD	PRO	556	80.094	16.804	3.304	1.00	18.93
ATOM	4300	CA	PRO	556	78.860	17.045	5.378	1.00	23.45
MOTA	4301	CB	PRO	556	77.943	16.643	4.226	1.00	22.35
MOTA	4302	CG	PRO	556	78.889	15.931	3.261	1.00	24.94
ATOM	4303	C	PRO	556	78.806	16.019	6.503	1.00	26.66
MOTA	4304	0	PRO	556	79.488	14.984	6.464	1.00	27.76
ATOM	4305	N	LEU	557	78.006	16.324	7.522	1.00	29.14
MOTA	4307	CA	LEU	557	77.842	15.440	8.676	1.00	30.83
ATOM	4308	CB	LEU	557	77.173	16.181	9.842	1.00	28.40
MOTA	4309	CG	LEU	557	76.775	15.393	11.097	1.00	22.93
ATOM	4310	CD1	LEU	557	77.989	14.897	11.835	1.00	23.02
ATOM	4311	CD2	LEU	557	75.970	16.285	11.984	1.00	23.53
ATOM	4312	c	LEU	557	77.028	14.200	8 321	1.00	31.04
MOTA	4313	Ō	LEU	557	75.968	14.293	7.694	1.00	31.89
ATOM	4314	N	TYR	558	77.552	13.041	8.700	1.00	29.88
ATOM	4316	CA	TYR	558	76.891	11.773	8.460	1.00	27.80
ATOM	4317	CB	TYR	558	77.741	10.878	7.562	1.00	28.04
ATOM	4318	CG	TYR	558	77.895	11.339	6.122	1.00	29.98
ATOM	4319	CD1	TYR	558	78.843	10.751	5.289	1.00	31.81
ATOM	4320	CE1	TYR	558	78.980	11.140	3.956	1.00	32.22
ATOM	4321	CD2	TYR	558	77.086	12.335	5.584	1.00	31.50
ATOM	4322	CE2	TYR	558	77.214	12.729	4.256	1.00	31.57
ATOM	4323	CZ	TYR	558	78.166	12.125	3.449	1.00	32.04
ATOM	4324	OH	TYR	558	78.317	12.511	2.134	1.00	33.34
ATOM	4326	C:	TYR	558	76.715	11.099	9.809	1.00	27.34
MOTA	4327	0	TYR	558	. 77.678	10.937	10.558	1.00	25.80
ATOM	4328	N	VAL	559	75.464	10.798	10.147	1.00	28.06
MOTA	4330	CA	VAL	559	75.118	10.118	11.394	1.00	26.67
ATOM	4331	CB	VAL	559	73.930	10.816	12.129	1.00	26.22
ATOM	4332	CG1	VAL	559	73.590	10.079	13.425	1.00	22.58
ATOM	4333	CG2	VAL	559	74.298	12.278	12.440	1.00	23.09
ATOM	4334	С	VAL	559	74.745	8.715	10.943	1.00	24.32
ATOM	4335	0	VAL	559	73.665	8.464	10.412	1.00	26.37
MOTA	4336	N	ILE	560	75.689	7.815	11.095	1.00	23.63
ATOM	4338	CA	ILE	560	75.514	6.448	10.664	1.00	24.67
MOTA	4339	СВ	ILE	560	76.901	5.859	10.299	1.00	24.62
ATOM	4340	CG2	ILE	560	76.753	4.507	9.646	1.00	30.13
MOTA	4341	CG1	ILE	560	77.627	6.810	9.326	1.00	21.87
ATOM	4342	CD1	ILE	560	79.114	6.538	9.162	1.00	22.25
ATOM	4343	С	ILE	560	74.814	5.621	11.737	1.00	27.30
						- ·			

A	rom 4	344	0	TTD	5.5.0					
A		345		ILE	560	, , , ,		505 12.8	65 1.0	0 28.80
	-	347		VAL	561			90 11.4		
	_	348		VAL	561			72 12.3		00
		349		VAL	561	71.57	<sup>7</sup> 2 4.9			
AT	_	350		VAL	561	71.86	6.2			
AT			_	/AL	561	70.67		54 11.6		_
AT			_	AL	561	72.57	2 2.9			
AT				/AL	561	72.85	3 2.6.			
ATO				LU	562	71.99	8 2.03			
ATO		_		LU	562	71.60	5 0.68			
ATO				LU	562	71.09	0.06			
ATO				LU	562	72.170	0.39			
ATC		`		LU	562	71.64	-0.96			
ATO				LU	562	72.389				
ATO				LU	562	70.491		-	_	
ATO				ւս	562	70.529		_	_	
ATO			٠.	'n	562	69.581				
			T	(R	563	70.666			_	32.53
ATO			A T	'R	563	69.699		_		30.70
ATO			в ту	R	563	70.419				30.65
ATO		_	G TY	'n	563	69.510				30.83
ATON			D1 TY	R	563	68.545				32.10
ATON			E1 TY	R	563	67.715	0.018		_ : ., 0	33.24
ATOM			D2 TY	_	563	69.609	-0.22			34.65
ATOM		1 CH	E2 TY		563	68.779	-2.098			31.04
ATOM		2 C2	TY:		563	67.831	-2.353			33.12
ATOM		3 OF	TY		563	67.902	-1.413	-		34.22
ATOM	,	5 C	TY		563	68.592	-1.650		1.00	34.76
ATOM	437	6 U	TY		563		-1.223		1.00	34.39
MOTA		7 N	ALA		64	68.855	-2.325	9.884	1.00	34.87
ATOM		9 CA			64	67.356	-0.861	9.091	1.00	35.49
ATOM	4380	СВ			64	66.212 65.213	-1.726	9.324	1.00	35.41
ATOM	4381	L C	ALA		64		-1.000	10.210	1.00	35.93
ATOM	4382	2 0	ALA		64	65.585	-2.056	7.962	1.00	37.19
MOTA	4383	N	SER	_	65	64.789	-1.276	7.434	1.00	38.08
ATOM	4385	CA	SER	-	65	65.931	-3.211	7.401	1.00	37.14
ATOM	4386	CB	SER		65	65.433	-3.616	6.080	1.00	36.83
ATOM	4387	OG	SER		65	66.151	-4.881	5.614	1.00	35.24
ATOM	4389	C	SER		65	66.105	-5.873	6.619	1.00	34.96
ATOM	4390	0	SER		55 55	63.932	-3.782	5.886	1.00	38.65
ATOM	4391	N	LYS		56	63.428	-3.617	4.760	1.00	37.80
ATOM	4393	CA	LYS		56	63.212	-4.077	6.964		38.96
ATOM	4394	CB	LYS	56		61.772	-4.271	6.851		37.83
ATOM	4395	CG	LYS	56		61.357	-5.495	7.655		39.07
ATOM	4396	CD	LYS			61.954	-6.765	7.078		43.73
ATOM	4397	CE	LYS	56		61.813	-7.950	7.996		47.07
ATOM	4398	NZ		56		62.258	-9.216	7.299		47.77
ATOM	4402	C	LYS	56		62.361	-10.326	8.278		
ATOM	4403		LYS	56		60.899	-3.050	7.165		51.48
ATOM	4404	O N	LYS	56		59.702	-3.180	7.442		37.53
ATOM	4404	N Cr	GLY	56		61.496	-1.866	7.066		38.55
ATOM	4407	CA	GLY	56		60.788	-0.627	7.305	_	35.23
ATOM		C	GLY	56		60.120	-0.485	8.656	• • -	3.64
ATOM	4408	0	GLY	56	7	60.518	-1.133			3.24
01-1	4409	N	ASN	568		59.120	0.389			3.80
SSSD/55	145 vni						-	0.740	1.00 з	1.65

MOTA	4411	CA	ASN	568	58.407	0.623	9.952	1.00	33.38
MOTA	4412	CB	ASN	568	57.831	2.055	10.025	1.00	37.10
MOTA	4413	CG	ASN	568	56.624	2.272	9.116	1.00	37.78
MOTA	4414	OD1	ASN	568	55.552	1.708	9.337	1.00	41.15
ATOM	4415	ND2	ASN	568	56.780	3.147	8.124	1.00	35.74
ATOM	4418	C	ASN	568	57.357	-0.435	10.263	1.00	33.33
MOTA	4419	0	ASN	568	56.917	-1.178	9.384	1.00	32.54
MOTA	4420	N	LEU	569	56.971	-0.490	11.532	1.00	33.35
MOTA	4422	CA	LEU	569	56.004	-1.455	12.040	1.00	32.38
ATOM	4423	CB	LEU	569	55.838	-1.263	13.552	1.00	27.50
ATOM	4424	CG	LEU	569	54.954	-2.259	14.291	1.00	26.34
ATOM	4425	CD1	LEU	569	55.452	-3.671	14.007	1.00	24.19
MOTA	4426	CD2	LEU	569	54.968	-1.951	15.787	1.00	21.44
MOTA	4427	С	LEU	569	54.641	-1.433	11.355	1.00	33.35
ATOM	4428	0	LEU	569	54.060	-2.484	11.095	1.00	34.99
ATOM	4429	N	ARG	570	54.130	-0.239	11.083	1.00	34.36
ATOM	4431	CA	ARG	570	52.827	-0.091	10.445	1.00	36.82
ATOM	4432	CB	ARG	570	52.548	1.393	10.188	1.00	37.28
ATOM	4433	CG	ARG	570	51.210	1.689	9.539	1.00	43.90
ATOM	4434	CD	ARG	570	51.212	3.099	8.967	1.00	50.39
ATOM	4435	NE	ARG	570	52.273	3.268	7.973	1.00	54.99
ATOM	4437	CZ	ARG	570	<b>5</b> 3.075	4.328	7.887	1.00	54.96
MOTA	4438	NH1	ARG	570	52.947	5.343	8.735	1.00	54.71
ATOM	4441	NH2	ARG	570	54.030	4.357	6.966	1.00	56.12
ATOM	4444	C	ARG	570	52.818	-0.877	9.133	1.00	36.53
ATOM	4445	0	ARG	570	51.968	-1.737	8.909	1.00	34.68
ATOM	4446	N	GLU	571	53.830	-0.611	8.320	1.00	37.14
ATOM	4448	CA	GLU	571	53.994	-1.253	7.031	1.00	37.94
MOTA	4449	CB	GLU	571	55.126	-0.558	5.274	1.00	39.71
ATOM	4450	CG	GLU	571	54.834	0.916	6.062	1.00	44.69
ATOM	4451	CD	GLU	571	55.934	1.665	5.346	1.00	52.22
ATOM ATOM	4452 4453	OE1 OE2	GLU	571	57.098	1.196	5.358	1.00	54.87
ATOM	4454	C C	GLU	571 571	55.629	2.743	4.777	1.00	56.37
ATOM	4455	0	GLU	571	54.258	-2.744	7.164	1.00	36.53
MOTA	4456	N	TYR	572	53.692 55.105	-3.550	6.426	1.00	36.35
ATOM	4458	CA	TYR	572	55.456	-3.105	8.120	1.00	35.77
ATOM	4459	CB	TYR	572	56.446	-4.499	8.371 9.534	1.00	36.28
ATOM	4460	CG	TYR	572	56.859	-4.555 -5.925	10.006	1.00	30.27
ATOM	4461	CD1	TYR	572	57.889	-6.626		1.00	31.65
ATOM	4462	CE1	TYR	572	58.354	-7.839	9.371 9.883	1.00	29.40
ATOM	4463	CD2	TYR	572	56.292	-6.480	11.161	1.00	29.32
ATOM	4464	CE2	TYR	572	56.749	-7.696	11.181	1.00	35.17
ATOM	4465	CZ	TYR	572	57.780	-8.366	11.038	1.00	33.08
ATOM	4466	ОН	TYR	572	58.234	-9.559	11.558		35.15
ATOM	4468	C	TYR	572	54.189	-5.321	8.672	1.00	36.91
ATOM	4469	0	TYR	572	53.942	-6.369	8.068		37.70
ATOM	4470	N	LEU	573	53.368	-4.799	9.576	1.00	36.82
ATOM	4472	CA	LEU	573	52.126	-5.442	9.970	1.00	37.64
ATOM	4473	CB	LEU	573	51.497	-4.659	11.122	1.00	36.03
ATOM	4474	CG	LEU	573	52.257	-4.641	12.445	1.00	36.17
ATOM	4475	CD1	LEU	573	51.590	-3.665	13.412	1.00	36.39
ATOM	4476	CD2	LEU	573	52.311	-6.042	13.412	1.00	36.17
ATOM	4477	C	LEU	573	51.117	-5.562	8.822	1.00	32.13 36.33
		-					0.944	4.00	בב.טב

A	TOM 4	478	0	LEU	573		4						
		479	N	GLN		•		-6.		8.6	49 1	.00	35.19
A	TOM 4	481	CA	GLN	574	50		-4.		8.0		00	37.66
		482.		GLN	574	50.0		-4.		6.9		CO	41.78
A.	TOM 4			GLN	574			-3.1		6.4		00	43.82
A.	TOM 4			GLN		48.8		-2.2		7.26		00	45.42
Al	rom 4			GLN	574	48.8		-0.8		6.80		00	49.56
AT				GLN	574	49.4		-0.5	06	5.77			
ΓA			_	GLN	574	48.2		0.0	01	7.56			52.22
ΓA				SLN	574	50.4		~5.4	27	5.78			54.86
AT		91 1	_ `	LA.	574	49.5		~5.8	98	5.04			42.89
AT				LA	575	51.6		-5.6	46	5.59			46.15
AT			-		575	52.16		-6.5	16	4.53			42.39
AT	<b>.</b>	95 C		LA	575	53.59		-6.16		4.17			40.19
ATO		_		LA	575	52.08		-7.97		4.97			40.68
ATO		_		LA	575	52.43		-8.86		4.210			40.49
ATO				RG	576	51.63		-8.19		6.202			43.34
ATO		_	_	RG	576	51.53	8	-9.54		6.761			38.76
ATC				RG	576	52.60		-9.70		7.846			38.44
ATC			_	RG	576	53.99		-9.60		7.284			34.26
ATO				RG	576	55.05	2	-9.62		8.356			37.16
ATO				RG	576	56.38		- 9.66		7. <b>7</b> 60		_	36.38
АТО					576	56.89°	7	-8.71		5.983			36.98
ATO					576	56.204	1	-7.61		5.689	1.00		38.62
ATO					576	58.112		-8.86		.491			11.41
ATO		_	AR		576	50.165		9.860		7.321	1.00		7.48
ATO		-	AR		576	50.013		10.746		1.169	1.00		0.55
ATON			AR		577	49.156		-9.146	_		1.00	-	3.20
ATON		•			577	47.794		-9.372		.844	1.00	_	1.98
ATOM			AR	_	577	46.896		-8.226		. 851	1.00		3.12
ATOM			AR	_	577	47.206		-6.910		.525	1.00		4.21
ATOM			ARG		77	46.402		-5.766		.941	1.00		5.21
ATOM		_	ARC	_	77	46.172		-4.734		. 948	1.00		7.50
ATOM			ARC	_	77	45.447		-3.641		.752	1.00		7.58
ATOM				_	<b>7</b> 7	44.882		-3.421		. 752 . 574	1.00		7.63
ATOM				_	77	45.256		-2.789		.747	1.00		0.05
ATOM		_	ARG		77	47.241	- 1	10.715		821	1.00		88.
ATOM	4531	-	ARG		77	47.297	~ 1	1.015		627	1.00		.10
ATOM	4533	N	GLN		94	53.448	- 1	3.666		976	1.00		.86
ATOM		CA	GLN		94	52.231		3.872		759	1.00		.97
ATOM	4534 4535	СВ	GLN			51.419		5.042		200	1.00		.30
ATOM		C	GLN	59		52.582	~1	4.116	10.		1.00		. 44
ATOM	4536	0	GLN	59		53.162	- 1	5.145			1.00		.02
ATOM	4537	N	LEU	59		52.218	- 1	3.151	10.		1.00		. 47
ATOM	4539	CA	LEU	59	5	52.499	- 1	3.187	11.		1.00		. 86
	4540	CB	LEU	59	5	52.597	- 7	1.751	12.4		1.00		. <b>7</b> 7
ATOM	4541	CG	LEU	59	5	53.471	-10	0.905	12.		1.00	59.	
ATOM ATOM	4542	CD1	LEU	59	5	53.307	_ (	9.427	12.0		1.00	61.	70
	4543	CD2	LEU	59	5	54.923	~11	1.324	12.3		1.00	64.	
ATOM	4544	С	LEU	59	5.	51.482		3.985	12.1		1.00	62.	
ATOM	4545	0	LEU	59		50.302			13.2		1.00	57.	49
ATOM	4546	N	SER	596		51.969		.026	12.9		1.00	56.	
ATOM	4548	CA	SER	596		51.369		.647	14.3		1.00	55.	
ATOM	4549	CB	SER	596		51.134		.447	15.2		.00	54.	
ATOM	4550	OG	SER	596		52.871	-16	.669	15.7		.00	55.	
						-2.0/1	- TP	.309	16.6	98 1		54.	

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	MOTA	4552	С	SER	596	50.723	-14.597	16.415	1.00	54.73
	ATOM	4553	0	SER	596	51.348	-13.579	16.704	1.00	53.29
	ATOM	4554	N	SER	597	49.704	-15.051	17.137	1.00	55.09
	MOTA	4556	CA	SER	597	49.215	-14.337	18.307	1.00	56.44
2	ATOM	4557	CB	SER	597	48.178	-15.185	19.044	1.00	59.14
	MOTA	4558	OG	SER	597	47.455	-16.009	18.138	1.00	65.57
	MOTA	4560	С	SER	597	50.387	-14.026	19.238	1.00	55.64
1	ATOM	4561	0	SER	597	50.430	-12.966	19.856	1.00	56.04
2	ATOM	4562	N	LYS	598	51.345	-14.948	19.315	1.00	54.91
2	MOTA	4564	CA	LYS	598	52.528	-14.773	20.161	1.00	54.25
1	MOTA	4565	CB	LYS	598	53.287	-16.096	20.311	1.00	54.23
i	ATOM	4566	CG	LYS	598	54.236	-16.138	21.494	1.00	55.12
7	MOTA	4567	CD	LYS	598	55.009	-17.448	21.523	1.00	59.41
i	MOTA	4568	CE	LYS	598	55.711	-17.679	22.858	1.00	58.10
i	MOTA	4569	NZ	LYS	598	54.750	-17.983	23.959	1.00	56.10
. 1	MOTA	4573	C	LYS	598	53.439	-13.716	19.536	1.00	52.32
1	MOTA	4574	0	LYS	598	53.986	-12.869	20.249	1.00	52.23
1	MOTA	4575	N	ASP	599	53.573	-13.768	18.208	1.00	47.57
7	MOTA	4577	CA	ASP	599	54.389	-12.818	17.466	1.00	45.47
7	MOTA	4578	CB	ASP	599 ·	54.324	-13.101	15.959	1.00	49.05
7	MOTA	4579	CG	ASP	599	55.245	-14.238	15.525	1.00	54.16
7	MOTA	4580	OD1	ASP	599	56.242	-14.503	16.223	1.00	61.34
2	MOTA	4581	OD2	ASP	599	54.992	-14.863	14.471	1.00	55.80
2	MOTA	4582	C	ASP	599	53.933	11.383	17.721	1.00	43.55
2	MOTA	4583	0	ASP	599	54.762	-10.491	17.895	1.00	44.34
7	MOTA	4584	N	LEU	600	52.622	-11.160	17.751	1.00	39.73
7	MOTA	4586	CA	LEU	600	52.104	-9.82.	17.989	1.00	37.64
Z	MOTA	4587	CB	LEU	600	50.597	-9.743	17.719	1.00	35.42
7	MOTA	4588	CG	LEU	600	50.075	9.951	16.287	1.00	33.95
7	MOTA	4589	CD1	LEU	600	48.621	-9.552	16.262	1.00	36.59
Į	MOTA	4590	CD2	LEU	600	50.841	-9.139	15.265	1.00	28.40
7	MOTA	4591	C	LEU	600	52.429	-9.347	19.402	1.00	38.24
7	MOTA	4592	0	LEU	600	52.817	-8.193	19.590	1.00	38.28
	MOTA	4593	N	VAL	601	52.305	-10.235	20.391	1.00	38.77
	MOTA	4595	CA	VAL	601	52.610	-9.855	21.772	1.00	38.87
	MOTA	4596	CB	VAL	601	52.121	-10.906	22.812	1.00	38.03
	MOTA	4597	CG1	VAL	601	52.150	-10.303	24.223	1.00	36.21
	MOTA	4598	CG2	VAL	601	50.710	-11.332	22.504	1.00	39.07
	MOTA	4599	С	VAL	601	54.123	-9.662	21.887	1.00	38.98
	MOTA	4600	0	VAL	601	54.601	-8.757	22.580	1.00	39.93
	MOTA	4601	N	SER	602	54.861	-10.488	21.155	1.00	37.35
	MOTA	4603	CA	SER	602	56.311	-10.422	21.126	1.00	37.11
	MOTA	4604	CB	SER	602	56.853	-11.469	20.154	1.00	39.38
	MOTA	4605	OG	SER	602	58.265	-11.413	20.061	1.00	46.76
	MOTA	4607	C	SER	602	56.695	-9.020	20.664	1.00	35.43
	MOT	4608	0	SER	602	57.493	-8.339	21.315	1.00	35.01
		4609	N	CYS	603	56.091	-8.586	19.561	1.00	33.42
	MOT	4611	CA	CYS	603	56.329	-7.254	19.015	1.00	32.18
		4612	CB	CYS	603	55.449	-7.035	17.790	1.00	32.38
	MOTA	4613	SG	CYS	603	55.440	-5.365	17.123	0.50	35.11 PRT1
	MOTA	4614	C	CYS	603	56.074	-6.167	20.059	1.00	31.20
	MOTA	4615	0	CYS	603	56.862	-5.234	20.185	1.00	32.44
	TOM	4616	N	ALA	604	55.001	-6.321	20.828	1.00	29.74
A	MOTA	4618	CA	ALA	604	54.640	-5.363	21.872	1.00	32.26



ATO				LA 604	53.232	2 -5.67	5 22 41	2	
ATO	_	-	AI	LA 604	55.656				_
ATO	_	-	AI	A 604	55.933		_	_	· · <del>-</del>
ATO			TY	(R 605	56.186			_	33.49
ATO			Y TY	'R 605	57.176			_	35.56
ATC			TY.	R 605	57.447				35.49
ATC			TY	R 605	58.562				36.12
ATO			1 TY	R 605	58.415	-8.23		- <del>-</del>	34.75
ATO			1 TY	R 605	59.444	-8.499			34.30
ATO				R 605	59.773	-9.021			36.26
ATO				R 605	60.812	-9.288		=	37.39
ATO				R 605	60.641	-9.027			37.81
ATO			TY	R 605	61.662	-9.324			38.34
ATO		_	TY	R 605	58.475	-5.972			42.09
ATO			TYI	R 605	58.981	-5.171			34.98
ATON			GLI	√ 606	58.996	-6.247		1.00	35.83
ATOM			GLN	J 606	60.218	-5.620		1.00	33.99
ATOM		_	GLN	606	60.506	-6.111		1.00	33.60
ATOM			GLN	606	60.858	-7.584	20.894	1.00	31.37
ATOM			GLN	606	61.175	-8.015	20.786 19.354	1.00	32.05
ATOM	<b></b>			606	62.145	-7.558	18.754	1.00	30.33
ATOM			GLN	606	60.353	-8.895	18.810	1.00	30.84
ATOM		-	GLN	606	60.123	-4.079	22.321	1.00	33.75
ATOM		•	GLN	606	61.070	-3.390	22.702	1.00	34.86
ATOM			VAL	607	58.975	-3.555	21.904	1.00	37.54
ATOM ATOM			VAL	607	58.748	-2.114	21.904	1.00	32.89
ATOM			VAL	607	57.425	-1.777	21.120	1 00	30.80
ATOM	4652		VAL	607	57.121	-0.299	21.120	1.00	28.82
ATOM	4653		VAL	607	57.541	~2.204	19.661	1.00	25.36
ATOM	4654	C	VAL	607	58.747	-1.532	23.312		23.37
ATOM	4655	0	VAL	607	59.359	-0.485	23.563		30.48
ATOM	4656 4658	N	ALA	608	58.106	-2.225	24.255		29.42
ATOM	4659	CA	ALA	608	58.064	-1.761	25.646		30.07
ATOM	4660	CB	ALA	608	57.027	-2.548	26.452		30.14 28.49
ATOM	4661	C	ALA	608	59.455	-1.849	26.305		31.25
ATOM	4662	0	ALA	608	59.791	-1.054	27.198		28.90
ATOM	4664	N	ARG	609	60.257	-2.819	25.870		31.61
ATOM	4665	CA CB	ARG	609	61.608	-2.979	26.393		31.99
ATOM	4666	CG	ARG	609	62.253	-4.245	25.856		34.93
ATOM	4667	CD	ARG	609	61.606	-5.507	26.317		0.82
MOTA	4668	NE	ARG	609	62.633	-6.606	26.397	_	2.68
ATOM	4670	CZ.	ARG	609	63.275	-6.621		_	3.85
ATOM	4671	NH1	ARG	609	64.332	-7.364			4.73
ATOM	4674	NH2	ARG	609	64.889	-8.162			1.40
ATOM	4677	C	ARG	609	64.803	-7.341			4.85
ATOM	4678	0 -	ARG	609	62.459	-1.796			3.70
ATOM	4679	N	ARG	609	63.130	-1.174			5.94
ATOM	4681	CA	GLY	610	62.459	-1.511	<b>a</b>		1.22
ATOM	4682	CA	GLY	610	63.232	-0.391			7.21
ATOM	4683	0	GLY	610	62.819				5.81
ATOM	4684	N	GLY	610	63.665				5.21
ATOM	4686	CA	MET	611	61.511				7.12
ATOM	4687		MET	611	60.969				3.82
-	,	-5	MET	611	59.457				9.29

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A	TOM	4688	CG	MET	611	59.004	2.706	24.135	1.00	31.07
A	TOM	4689	SD	MET	611	59.732	4.286	23.617	1.00	28.38
A	TOM	4690	CE	MET	611	59.155	5.431	24.922	1.00	28.34
A'	TOM	4691	С	MET	611	61.341	2.261	27.178	1.00	30.34
A'	TOM	4692	0	MET	611	61.596	3.334	27.730	1.00	31.73
A'	TOM	4693	N	GLU	612	61.347	1.109	27.837	1.00	32.72
A'	TOM	4695	CA	GLU	612	61.723	1.057	29.253	1.00	35.46
A'	TOM	4696	СВ	GLU	612	61.603	-0.370	29.792	1.00	34.70
A'	TOM	4697	CG	GLU	612	62.029	-0.516	31.237	1.00	32.31
A'	TOM	4698	CD	GLU	612	62.135	1.968	31.688	1.00	33.14
A'	TOM	4699	OE1	GLU	612	62.546	-2.834	30.883	1.00	30.79
A'	TOM	4700	OE2	GLU	612	61.826	-2.240	32.867	1.00	36.13
A'	TOM	4701	С	GLU	612	63.178	1.544	29.353	1.00	36.43
A'	TOM	4702	0	GLU	612	63.534	2.319	30.261	1.00	35.38
A'	TOM	4703	N	TYR	613	63.999	1.107	28.391	1.00	35.47
A'	TOM	4705	CA	TYR	613	65.403	1.507	28.334	1.00	33.16
A'	TOM	4706	CB	TYR	613	66.156	0.743	27.241	1.00	31.33
A'	TOM	4707	CG	TYR	613	67.612	1.146	27.132	1.00	33.03
A'	TOM	4708	CD1	TYR	613	68.584	0.544	27.931	1.00	36.69
A'	rom	4709	CE1	TYR	613	69.930	0.927	27.851	1.00	36.82
A'	TOM	4710	CD2	TYR	613	68.021	2.148	26.247	1.00	33.49
A.	TOM	4711	CE2	TYR	613	69.352	2.540	26.157	1.00	34.73
A'	TOM	4712	CZ	TYR	613	70.307	1.927	26.963	1.00	37.07
A'	rom	4713	OH	TYR	613	71.632	2.318	26.896	1.00	36.77
A.	ГОМ	4715	С	TYR	613	65.539	3.005	28.088	1.00	31.82
A.	rom	4716	С	TYR	613	66.256	3.682	28.814	1.00	34.75
A	rom	4717	N	LEU	614	64.836	3.536	27.090	1.00	28.44
ΑT	rom	4719	CA	LEU	614	64.931	4.956	26.793	1.00	25.67
A	rom	4720	CB	LEU	614	64.089	5.319	25.569	1.00	24.75
ΑT	rom	4721	CC	LEU	614	64.545	4.778	24.208	1.00	23.73
A.	rom	4722	CD1	LEU	614	63.594	5.257	23.125	1.00	20.54
A7	MOT	4723	CD2	LEU	614	65.983	5.213	23.894	1.00	23.21
A7	MOT	4724	C	LEU	614	64.499	5.761	28.001	1.00	28.30
	rom	4725	0	LEU	614	65.110	6.770	28.345	1.00	27.09
	rom	4726	N	ALA	615	63.470	5.272	28.683	1.00	32.73
A	rom	4728	CA	ALA	615	62.955	5.945	29.871	1.00	34.10
	rom	4729	CB	ALA	615	61.625	5.314	30.314	1.00	33.68
	MO	4730	C	ALA	615	63.986	5.913	31.007	1.00	33.84
	MOT	4731	0	ALA	615	64.112	6.885	31.753	1.00	34.95
	MO	4732	N	SER	616	64.722	4.809	31.134	1.00	32.69
	rom	4734	CA	SER	616	65.738	4.703	32.175	1.00	33.50
	MOT	4735	CB	SER	616	66.287	3.277	32.285	1.00	28.27
	ГОМ	4736	OG	SER	616	67.076	2.935	31.165	1.00	25.54
	rom	4738	С	SER	616	66.870	5.678	31.865	1.00	35.43
	rom	4739	0	SER	616	67.637	6.061	32.755	1.00	37.32
	MOT	4740	N	LYS	617	66.971	6.060	30.592	1.00	34.80
	MO7	4742	CA	LYS	617	67.975	7.010	30.143	1.00	33.01
	МО	4743	CB	LYS	617	68.508	6.620	28.776	1.00	33.18
	MOT	4744	CG	LYS	617	69.224	5.302	28.797	1.00	35.64
	MOT	4745	CD	LYS	617	70.423	5.380	29.710	1.00	40.31
	MOT	4746	CE	LYS	617	71.075	4.025	29.863	1.00	43.03
	MOT	4747	NZ	LYS	617	72.426	4.152	30.449	1.00	45.54
	MOT	4751	C	LYS	617	67.360	8.397	30.102	1.00	32.87
ΓA	MOT	4752	0	LYS	617	67.892	9.308	29.470	1.00	34.06

	ATOM	4753	N	IVC								
	ATOM	4755	CA	LYS				8.	542 30	. 772	1 0 0	
	3 5000	4756		LYS	618		00			.872	1.00	
		4757	CB	LYS	618	66.3	84	10.8			1.00	33.28
		4758	CG	LYS	618	66.9		10.3		558	1.00	37.22
		1759	CD	LYS	618	65.9		10.2		869	1.00	43.11
			CE	LYS	618	66.5	20	9.6		957	1.00	49.82
		760		LYS	618	65.6	59			199	1.00	55.20
		764		LYS	618	65.0		9.8		415	1.00	61.31
		765	0	LYS	618	64.69		10.3		542	1.00	31.57
			N .	CYS	619	64.95		11.5			1.00	31.10
	m		CA (	CYS	619	64.51		9.50			1.00	31.04
			CB (	CYS	619			9.92		196	1.00	29.21
			SG (	:YS	619	65.21		9.06		125	1.00	28.55
			-	YS	619	64.78		9.40		192	1.00	26.31
		772 (	_	YS	619	62.99	9	9.84	9 27.0		1.00	
		773 N	_	LE	620	62.37		8.82	7 27.3		1.00	30.91
	OM 47	775 C				62.41	1 1	0.96	7 26.6		1.00	31.18
AT	OM 47				620	60.98		1.07	3 26.4			29.48
AT	OM 47		-		620	60.402	' 1	2.34			1.00	29.34
AT	OM 47				620	58.944	1	2.53			1.00	28.12
AT					620	60.521	1	2.26			1.00	28.76
AT					620	60.062		3.522			00	28.36
ATO					520	60.852	1:	1.188	24.90			25.55
ATO			II		520	61.254		2.193				30.97
ATO	•		HI		21	60.307		).147			.00	33.88
ATC				_	21	60.148		0.080		_	.00	31.55
ATO				_	21	59.721		.668			.00	31.85
ATO	-	_		s s	21	59.913			22.42		.00	88.27
ATO	- , ,	_		S 6	21	60.608		.373	20.97			4.68
ATO		_		S 6	21	59.354		.383	20.35			4.39
ATO				S 6:	21	59.691		.130	19.97			5.87
ATO			2 HI		21	60.444		.623				7.65
			HIS	62	21	59.187		.571	19.00			5.80
ATO	_		HIS			59.387		. 096	22.224			4.38
ATON			ARG			58.080		539	21.104	1.		8.74
ATOM	- , 5 ,	CA	ARG			57.093		374	22.898	1.		7.17
ATOM		CB	ARG	62				346	22.425	1.		7.27
ATOM		CG	ARG			57.718		746	22.298		_	3.63
ATOM	•	CD	ARG			58.261		271	23.601	1.0		). <b>4</b> 7
ATOM		NE	ARG	62		58.661	15.		23.530	1.0		.76
ATOM		CZ	ARG	62		59.129	16.	174	24.842	1.0		
ATOM		NH1	ARG	62:		60.299	15.	821	25.375	1.0		.09
ATOM		NH2	ARG	622		61.132	15.0		24.699	1.0		.86
MOTA	4810	C	ARG			60.606	16.	167	26.624	1.0		.20
ATOM	4811	0	ARG	622		56.324	11.9		21.151	1.0		.19
ATOM	4812	N	ASP	622		55.300	12.6	14	20.867	1.0		. 23
ATOM	4814	CA		623		56.805	11.0		20.364			45
ATOM	4815		ASP	623		56.075	10.6		19.160	1.0		
ATOM	4816	CB	ASP	623	!	56.581	11.4			1.00		
ATOM	4817	CG	ASP	623		55.635	11.2		17.910	1.00	•	
ATOM		OD1	ASP	623	9	6.077	11.4		16.687	1.00	•	
ATOM	4818	OD2	ASP	623	9	4.445	10.8		15.538	1.00	49.	
ATOM	4819	C	ASP	623	5	6.126			16.872	1.00	49.	
ATOM	4820	0	ASP	623		6.325	9.1		18.967	1.00	33.	
	4821	N	LEU	624		5.999	8.6		17.864	1.00	31.	
ATOM	4823	CA	LEU	624		6.014	8.40		0.059	1.00		
CCC ~ :-					J	~.U14	6.95	4 1	.9.950	1.00		
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ATOM	1 4824	CB	LEU	624	55.983	6.307	21.342	1.00	27.43	
ATOM	1 4825	CG	LEU	624	55.949	4.778	21.441	1.00	28.69	
ATOM	1 4826	CD1	LEU	624	57.139	4.132	20.731	1.00	24.75	
ATOM	1 4827	CD2	LEU	624	55.927	4.389	22.894	1.00	27.39	
ATOM	1 4828	С	LEU	624	54.803	6.532	19.109	1.00	31.22	
ATOM	1 4829	0	LEU	624	53.680	6.952	19.380	1.00	33.44	
ATOM	1 4830	N	ALA	625	55.053	5.763	18.054	1.00	28.85	
ATOM	4832	CA	ALA	625	54.009	5.286	17.159	1.00	26.93	
ATOM	4833	CB	ALA	625	53.559	6.400	16.227	1.00	25.03	
ATOM	4834	C	ALA	625	54.642	4.162	16.356	1.00	28.44	
ATOM	4835	0	ALA	625	55.863	4.065	16.317	1.00	31.32	
ATOM	4836	N	ALA	626	53.828	3.329	15.705	1.00	29.14	
ATOM	4838	CA	ALA	626	54.344	2.205	14.905	1.00	28.42	
ATOM	4839	CB	ALA	626	53.192	1.357	14.353	1.00	27.37	
ATOM	4840	C	ALA	626	55.231	2.698	13.771	1.00	26.38	
ATOM	4841	0	ALA	626	56.195	2.041	13.395	1.00	26.12	
ATOM	4842	N	ARG	627	54.890	3.861	13.230	1.00	27.16	
ATOM	4844	CA	ARG	627	55.669	4.474	12.158	1.00	28.44	
ATOM	4845	СВ	ARG	627	55.022	5.794	11.733	1.00	28.19	
ATOM	4846	CG	ARG	627	54.889	6.793	12.867	1.00	30.34	
ATOM	4847	CD	ARG	627	54.456	8.155	12.361	1.00	34.08	
ATOM	4848	NE	ARG	627	54.081	9.024	13.471	1.00	35.58	
ATOM	4850	CZ	ARG	627	52.849	9.123	13.950	1.00	35.55	
ATOM	4851	NH1	ARG	627	51.860	8.422	13.420	1.00	35.67	
ATOM	4854	NH2	ARG	627	52.618	9.898	14.993	1.00	40.81	
ATOM	4857	С	ARG	527	57.108	4.733	12.630	1.00	28.06	
ATOM	4858	0	ARG	627	58.044	4.737	11.825	1.00	29.80	
MOTA	4859	N	ASN	628	57.272	4.935	13.940	1.00	28.50	
MOTA	4861	CA	ASN	628	58.582	5.195	14.544	1.00	26.14	
ATOM	4862	CB	ASN	628	58.494	6.340	15.551	1.00	23.55	
ATOM		CG	ASN	628	58.319	7.681	14.874	1.00	27.48	
MOTA		OD1	ASN	628	58.874	7.919	13.800	1.00	34.12	
ATOM		ND2	ASN	628	57.543	8.556	15.479	1.00	23.21	
ATOM		С	ASN	628	59.263	3.965	15.153	1.00	26.76	
MOTA		0	ASN	628	60.202	4.078	15.948	1.00	26.90	
ATOM		N	VAL	629	58.774	2.794	14.767	1.00	27.02	
MOTA		CA	VAL	629	59.344	1.523	15.186	1.00	27.81	
ATOM		CB	VAL	629	58.298	0.622	15.864	1.00	26.83	
ATOM	4874	CG1	VAL	629	58.876	-0.766	16.115	1.00	20.74	
ATOM		CG2	VAL	629	57.836	1.259	17.165	1.00	22.49	
ATOM		C	VAL	629	59.781	0.895	13.861	1 00	28.61	
ATOM		0	VAL	629	58.983	0.809	12.924	1.00	28.76	
ATOM		N	LEU	630	61.059	0.557	13.746	1.00	30.35	
ATOM		CA	LEU	630	61.576	-0.033	12.514	1.00	32.42	
ATOM		CB	LEU	630	62.824	0.725	12.040	1.00	32.28	
ATOM		CG	LEU	630	62.697	2.249	11.880	1.00	27.75	
ATOM	4883	CD1	LEU	630	64.019	2.860	11.469	1.00	24.71	
ATOM	4884	CD2	LEU	630	61.611	2.582	10.872	1.00	27.70	
ATOM	4885	C	LEU	630	61.895	-1.488	12.799	1.00	32.89	
ATOM		0	LEU	630	62.167	-1.838	13.943	1.00	32.32	
ATOM		N	VAL	631	61.831	-2.336	11.774	1.00	34.81	
MOTA		CA	VAL	631	62.087	-3.772	11.943	1.00	33.87	
ATOM		CB	VAL	631	60.818	-4.616	11.597	1.00	31.60	
ATOM	4891	CG1	VAL	631	60.929	-6.004	12.197	1.00	30.84	

AΊ	OM 4	100 6								
				JAL		59.54	5 -3.9	16 12.0	89 1.0	00 05
				/AL	631	63.28	6 -4.2			
			_ `	AL	631	63.36	5 -4.0			
AT				HR	632	64.21	5 -4.9			
AT				HR	632	65.418	8 -5.4		_	
AT				HR	632	66.54	-5.7			
ATO		_		HR	632	66.187	7 -6.8			
•	OM 49			HR	632	66.750	-4.4			
ATO				HR	632	65.162	-6.7			
ATO				HR	632	64.078	-7.30			
ATO				LU	633	66.153	-7.12			
ATO				T.O.	633	66.030	-8.33			
ATO				בט	633	67.314	-8.60			
ATO					633	67.205	-9.76			
ATO					633	66.380	-9.44			
ATO					633	65.637	-8.43			
ATO					633	66.479	-10.22			
ATO		_	GL		533	65.708	-9.52			
ATO			GL		533	64.974	-10.42			50
ATO		_	AS		534	66.201	-9.49			
ATON	_		AS		34	65.961	-10.58			_ <del>-</del>
ATON		_	AS.		34	67.221	-10.86			44.23
ATOM			AS:		34	68.443	-11.181			50.17
ATOM					34	68.363	-12.113	10.857		56.79 59.62
ATOM	1 4921		ASI ASI	_	34	69.482	-10.490	11.837		58.62
ATOM		-	ASI		34	64.756	-10.331	12.644		43.26
ATOM		_	ASN		34	64.652	-10.879	13.733		43.58
ATOM			ASN	_	35	63.858	-9.475	12.165		43.36
ATOM	4926		ASN	_	35	62.612	-9.126	12.847		43.66
ATOM	4927		ASN	_	35	61.698	-10.355	12.930	1.00	46.94
ATOM	4928		ASN		35 35	61.413	-10.958	11.572	1.00	48.19
ATOM	4929	ND2	ASN		35	60.831	-10.314	10.702	1.00	51.42
ATOM	4932	C	ASN		35	61.832	-12.198	11.380	1.00	49.44
ATOM	4933	0	ASN	63		62.694 61.774	-8.463	14.216	1.00	43.03
ATOM	4934	N	VAL	63		63.763	-8.596	15.031	1.00	43.03
ATOM	4936	CA	VAL	63		63.915	-7.712	14.467	1.00	42.69
ATOM	4937	CB	VAL	63		65.406	-7.034	15.756	1.00	38.30
ATOM	4938	CG1	VAL	63		65.555	-6.861	16.134	1.00	37.92
ATOM	4939	CG2	VAL	63		66.052	-6.040	17.421	1.00	37.14
ATOM	4940	C	VAL	63		63.251	-8.226	16.306	1.00	37.55
ATOM	4941	0	VAL	63		63.486	-5.673 -4.926	15.688	1.00	35.75
ATOM	4942	N	MET	63		62.355		14.746	1.00	36.28
ATOM	4944	CA	MET	63		61.672	-5.396 -4.103	16.628	1.00	34.73
MOTA	4945	CB	MET	63		60.456	-4.103 -4.152	16.680	1.00	33.22
ATOM	4946	CG	MET	63		59.364		17.608	1.00	34.83
ATOM	4947	SD	MET	63		58.661	-5.148	17.231	1.00	34.41
ATOM	4948	CE	MET	63		58.869	-4.926	15.589	1.00	33.19
ATOM	4949	C	MET	631		62.677	-6.584	14.913	1.00	29.73
ATOM	4950	0	MET	637		63.281	-3.107	17.250	1.00	33.75
ATOM	4951	N	LYS	638		62.839	-3.357	18.308	1.00	31.79
ATOM	4953	CA	LYS	638		63.774	-1.980	16.558	1.00	31.83
ATOM	4954	CB	LYS	638		64.986	-0.939	16.965	1.00	28.17
ATOM	4955	CG	LYS	638		66.006	-0.930 -1.967	16.038	1.00	24.98
							<b>4.70</b> /	16.400	1.00	23.17
55SD/55	145 v01									

ATOM	4956	CD	LYS	638	67.193	-1.916	15.470	1.00	25.04
ATOM	4957	CE	LYS	638	68.212	-2.969	15.847	1.00	24.79
ATOM	4958	NZ	LYS	638	68.747	-2.765	17.220	1.00	24.91
ATOM	4962	C	LYS	638	63.165	0.445	16.986	1.00	26.04
MOTA	4963	0	LYS	638	62.803	0.958	15.936	1.00	24.44
ATOM	4964	N	ILE	639	63.052	1.031	18.181	1.00	25.14
MOTA	4966	CA	ILE	639	62.508	2.376	18.351	1.00	25.68
ATOM	4967	CB	ILE	639	62.589	2.863	19.839	1.00	27.40
MOTA	4968	CG2	ILE	639	61.875	4.189	19.984	1.00	18.94
MOTA	4969	CG1	ILE	639	62.019	1.827	20.826	1.00	26.05
ATOM	4970	CD1	ILE	639	60.517	1.667	20.792	1.00	25.07
ATOM	4971	C	ILE	639	63.387	3.338	17.543	1.00	25.82
ATOM	4972	0	ILE	639	64.619	3.283	17.642	1.00	25.76
MOTA	4973	N	ALA	640	62.758	4.231	16.783	1.00	25.92
MOTA	4975	CA	ALA	640	63.477	5.218	15.976	1.00	26.12
MOTA	4976	CB	ALA	640	63.222	4.964	14.506	1.00	26.54
ATOM	4977	C	ALA	640	63.042	6.643	16.344	1.00	26.33
ATOM	4978	0	ALA	640	61.996	6.828	16.974	1.00	26.20
MOTA	<b>49</b> 79	И	ASP	641	63.863	7.637	15.993	1.00	26.59
ATOM	4981	CA	ASP	641	63.545	9.052	16.245	1.00	28.09
ATOM	4982	CB	ASP	641	62.217	9.443	15.593	1.00	31.43
ATOM	4983	CG	ASP	641	62.346	9.762	14.107	1.00	36.81
MOTA	4984	OD1	ASP	641	63.409	9.478	13.500	1.00	40.24
ATOM	4985	OD2	ASP	641	61.356	10.299	13.548	1.00	40.49
MOTA	4986	C	ASP	641	63.455	9.442	17.700	1.00	28.40
ATOM	4987	О	ASP	641	62.825	10.446	18.041	1.00	29.30
MOTA	4988	N	PHE	642	64.080	8.658	18.564	1.00	30.27
ATOM	4990	CA	PHE	642	64.044	8.943	19.992	1.00	30.97
ATOM	4991	CB	PHE	642	64.327	7.664	20.787	1.60	24.64
ATOM	4992	CG	PHE	642	65.673	7.063	20.505	1.00	20.96
MOTA	4993	CD1	PHE	642	66.812	7.539	21.163	1.00	16.89
ATOM	4994	CD2	PHE	642	65.806	6.026	19.576	1.00	16.23
ATOM	4995	CE1	PHE	642	68.372	6.990	20.900	1.00	18.35
ATOM	4996	CE2	PHE	642	67.051	5.471	19.305	1.00	18.76
ATOM	4997	CZ	PHE	642	68.195	5.954	19.970	1.00	17.91
ATOM	4998	C	PHE	642	65.024	10.045	20.414	1.00	34.53
ATOM	4999	0	PHE	642	64.990	10.503	21.563	1.00	35.23
MOTA	5000	N	GLY	643	65.910	10.433	19.500	1.00	36.40
MOTA MOTA	5002 5003	CA	GLY	643	66.888	11.455	19.799	1.00	38.28
ATOM	5003	С 0	GLY GLY	643	66.634	12.768	19.093	1.00	41.44
ATOM	5005	N		643	67.482	13.652	19.132	1.00	44.10
ATOM	5003	CA	LEU	644	65.461	12.921	18.484	1.00	45.44
ATOM	5007		LEU	644	65.131	14.144	17.748	1.00	49.14
MOTA	5009	CB CG	LEU	644	63.832	13.975	16.969	1.00	46.26
MOTA	5010		LEU	644	63.823	12.967	15.836	1.00	42.90
ATOM	5010	CD1 CD2	LEU	644	62.527	13.134	15.070	1.00	42.68
ATOM	5012	CD2	LEU	644	65.004	13.228	14.934	1.00	45.15
ATOM	5012	0	LEU LEU	644	65.027	15.396	18.605	1.00	53.90
MOTA	5013	N		644	64.488	15.356	19.715	1.00	56.54
ATOM	5014	CA	ALA	645	65.534	16.505	18.068	1.00	57.59
ATOM	5016	CB	ALA	645	65.505	17.794	18.759	1.00	60.15
ATOM	5017	СВ	ALA	645	66.539	18.741	18.156	1.00	59.55
ATOM	5019	0	ALA	645	64.112	18.407	18.667	1.00	61.90
	2013	U	ALA	645	63.393	18.500	19.663	1.00	63.83

			N į	ASP 65	2 52.09	90 22.19	1 14 00	_	
			CA 1	ASP 65				00	
	_		CB A	SP 65					89.75
			CG A	SP 65					88.08
AT	_		D1 A	SP 652					87.09
AT		26 (	DD2 A	SP 652					86.85
AT		27 C	: A	SP 652					86.69
AT(	OM 50	28 C	) A	SP 652					89.98
ATO		29 N		YR 653			_		90.19
ATO		31 C		YR 653				1.00	90.26
ATO	DM 50	32 C		YR 653		-		1.00	90.78
ATC	OM 50:			YR 653				1.00	91.65
ATC	M 50		D1 TY						93.43
ATO			El Ty			· ·	18.752		94.60
ATO					47.477		20.058		95.35
ATO					49.083		18.101	1.00	
ATO				_	49.558		19.406	1.00	93.46
ATO			_	_	48.748	20.435	20.378	1.00	94.36
ATO					49.220	20.554	21.669		95.26
ATO		_	TY		47.602	19.231	14.021	1.00	95.00
ATO		_	TY		47.045	18.131	14.012	1.00	90.47
ATON			TY		47.632	20.031	12.962	1.00	91.33
ATOM	- • •			R 654	46.954	19.673	11.727	1.00	39.21
ATOM				R 654	46.205	20.893	11.727	1.00	89.09
ATOM				₹ 654	45.275	21.499		1.00	88.23
				₹ 654	45.776	22.140	12.209	1.00	87.65
ATOM	<b></b>				44.929	22.655	13.343	1.00	86.76
ATOM			YYT S	654	43.895	21.396	14.312		87.17
ATOM			YYT S	654	43.032	21.912	12.067		88.61
ATOM			TYR	654	43.557		13.033	1.00	89.32
ATOM			TYR	654	42.710	22.538	14.153	1.00	88.66
ATOM	5055	C	TYR	654	47.857	23.034	15.117		89.35
ATOM	5056	0	TYR		47.396	19.080	10.651	1.00	29.49
ATOM	5057	N	LYS	655	49.139	18.772	9.552	1.00	38.37
ATOM	5059	CA	LYS	655	50.056	18.919	10.959	1.00	90.80
ATOM	5060	CB	LYS	655	51.508	18.356	9.982	1.00	93.18
ATOM	5061	CG	LYS	655	52.504	18.713	10.311		95.66
ATOM	5062	CD	LYS	655		18.133	9.315		9.82
ATOM	5063	CE	LYS	655	53.932	18.585	9.562	1.00103	. 58
ATOM	5064	NZ	LYS	655	54.898	17.833	8.637	1.00106	
ATOM	5068	С	LYS	655	56.325	18.246		1.00108	
ATOM	5069	0	LYS	655	49.884	16.847	9.935		3.56
ATOM	5070	N	LYS	656	49.904	16.182	10.972		3.72
ATOM	5072	CA	LYS	656	49.670	16.320			4.19
ATOM	5073	СВ	LYS		49.500	14.886			4.84
ATOM	5074	CG		656	48.628	14.620			4.64
ATOM	5075	CD	LYS	656	47.155	14.874			5.54
ATOM	5076		LYS	656	46.402	14.709			
ATOM	5077	CE	LYS	656	44.926	14.449		1.00101.	9.56
ATOM	5081	NZ	LYS	656	44.202	14.327			
ATOM		C	LYS	656	50.859	14.225	_	1.00103.	
ATOM	5082	0	LYS	656	51.823	14.878			.18
ATOM	5083	N	GLY	660	48.651	A	<b></b>		. 74
ATOM	5085	CA	GLY	660	47.932				.76
	5086	C	GLY	660	47.241	10			.04
ATOM	5087	0	GLY	660	46.183			_	. 90
						-+32	7.525 1	.00 53	. 92
SSSD/551	145 VA1								

ATOM	5088	N	ARG	661	47.838	10.243	8.328	1.00	51.87
MOTA	5090	CA	ARG	661	47.297	10.177	9.679	1.00	48.23
MOTA	5091	CB	ARG	661	47.755	8.891	10.377	1.00	49.74
ATOM	5092	CG	ARG	661	47.506	7.620	9.566	1.00	47.59
ATOM	5093	CD	ARG	661	47.561	6.390	10.446	1.00	51.85
MOTA	5094	NE	ARG	661	47.584	5.155	9.663	1.00	52.94
ATOM	5096	CZ	ARG	661	48.035	3.988	10.117	1.00	52.19
ATOM	5097	NHl	ARG	661	48.503	3.884	11.356	1.00	52.10
ATOM	5100	NH2	ARG	661	48.036	2.926	9.327	1.00	54.43
MOTA	5103	С	ARG	661	47.722	11.401	10.483	1.00	43.67
ATOM	5104	0	ARG	661	48.658	12.103	10.104	1.00	41.45
ATOM	5105	N	LEU	662	47.019	11.656	11.579	1.00	40.27
ATOM	<b>51</b> 07	CA	LEU	662	47.310	12.799	12.437	1.00	37.15
ATOM	5108	CB	LEU	662	46.021	13.533	12.783	1.00	37.39
MOTA	5109	CG	LEU	662	45.301	14.149	11.588	1.00	
ATOM	5110	CD1	LEU	662	43.852	14.428	11.937	1.00	35.38
ATOM	5111	CD2	LEU	662	46.041	15.407	11.163	1.00	39.79
ATOM	5112	С	LEU	662	47.973	12.330	13.716	1.00	34.68
ATOM	5113	0	LEU	662	47.327	11.718	14.568	1.00	33.33
ATOM	5114	N	PRO	663	49.260	12.655	13.892	100	34.11
ATOM	5115	CD	PRO	663	50.086	13.389	12.924	1.00	33.67
ATOM	5116	CA	PRO	663	50:052	12.281	15.068	1.00	33.55
ATOM	5117	CB	PRO	663	51.367	13.003	14.833	1.00	32.99
ATOM	5118	CG	PRO	663	51.479	12.966	13.328	1.00	36.09
MOTA.	5119	C	PRO	663	49.412	12.665	16.399	1.00	33.55
ATOM	5120	0	PRO	663	49.683	12.036	17.426	1.00	34.11
ATOM	5121	N	VAL	664	48.566	13.697	16.387	1.00	32.63
ATOM	5123	CA	VAL	664	47.874	14.092	17.613	1.00	32.24
MOTA	5124	CB	VAL	664	46.953	15.327	17.396	1.60	33.24
ATOM	5125	CG1	VAL	664	47.779	16.583	17.252	1.00	35.01
ATOM	5126	CG2	VAL	664	46.089	15.154	16.155	1.00	35.44
MOTA	5127	C	VAL	664	47.072	12.896	18.150	1.00	31.08
ATOM	5128	0	VAL	664	46.866	12.760	19.360	1.00	31.49
ATOM	5129	N	LYS	665	46.710	11.978	17.255	1.00	29.75
ATOM	5131	CA	LYS	665	45.956	10.788	17.638	1.00	28.83
MOTA	.5132	CB	LYS	665	45.411	20.083	16.397	1.00	29.52
MOTA	5133	CG	LYS	665	44.242	10.835	15.797	1.00	27.21
ATOM	5134	CD	LYS	665	43.905	10.431	14.397	1.00	27.25
ATOM	5135	CE	LYS	665	42.684	11.228	13.931	1.00	28.63
ATOM	5136	NZ	LYS	665	42.266	10.902	12.545	1.00	25.33
ATOM	5140	С	LYS	665	46.718	9.830	18.537	1.00	29.03
MOTA	5141	0	LYS	665	46.152	8.869	19.046	1.00	28.37
MOTA	5142	N	TRP	666	47.994	10.123	18.765	1.00	30.40
ATOM	5144	CA	TRP	666	48.825	9.296	19.628	1.00	31.10
ATOM	5145	CB	TRP	666	50.123	8.906	18.917	1.00	29.53
MOTA	5146	CG	TRP	666	49.946	7.781	17.966	1.00	27.03
MOTA	5147	CD2	TRP	666	49.407	7.853	16.638	1.00	25.06
MOTA	5148	CE2	TRP	666	49.418	6.546	16.116	1.00	23.83
ATOM	5149	CE3	TRP	666	48.924	8.899	15.835	1.00	26.08
MOTA	5150	CD1	TRP	666	50.257	6.475	18.186	1.00	20.75
MOTA	5151	NE1	TRP	666	49.937	5.729	17.086	1.00	24.92
ATOM	5153	CZ2	TRP	666	48.962	6.245	14.832	1.00	23.95
MOTA	5154	CZ3	TRP	666	48.466	8.604	14:548	1.00	29.09
ATOM	5155	CH2	TRP	666	48.491	7.282	14.060	1.00	29.22
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ATOM 5156 C TRP	
ATOM 5157 0	666 49.174 10.049 20.896 3.00
ATOM 5150	666 49 701 20.896 1.00 33 30
ATOM 5-0	667 48 863 21.849 1.00 34 30
CA MET A	667 11.340 20.910 1 00
MET 2	12.175 22 25
ATOM 5162 CG MEC	49.205 13.645 22 655
ATOM 5163 SD MP	50.475 14.047 20.001 1.00 40.08
ATOM 5164 CE	70' 50 556 4
ATOM 5165 C MET 6	067 50 957 3-1-1-20./13 1.00 57 31
ATOM FIGS MET 6	15.928 18.949 1 00
ME'I' 6	67 45 - 43.28/ 1 00 25
111011 5167 N ALA 64	68 11.871 23.195 1 00 37.81
AIOM 5169 CA AT	48.958 11.964 24 442
ATOM 5170 CB 777	48.286 11 846 35 1.00 36.47
ATOM 5171 C ALA 66	58 49 300 25./18 1.00 37 06
ATOM CITE ALA 66	58 47 549 26.835 1.00 35 76
- O ALA EE	58 40 13.161 25.893 1 00 15
2773 N PRO 66	14.201 25.414 1 00
ATOM 5174 CD PPO CC	13.142 26 520
ATOM 5175 CA DDG	45.819 11.981 27 200 41.60
ATOM 5176 CD	9 45 614 27.282 1.00 41 64
ATOM STORE PRO 669	9 44 470 20.841 1.00 43 25
ATOM 57-0 CG PRO 669	9 44 33 82/ 27.718 1 00 43
PRO 669	9 46 355 12.368 27.325 1 00 44.5
51/9 O PRO 660	15.486 27 526
ATOM 5180 N	46.304 16.644 37 74
ATOM 5182 CD 070	47.135 15.164 20 1.00 43.79
ATOM 5183 CP 670	47 905 28.580 1 00 44 29
ATOM FIRE	48 596 15 29.266 1.00 45 36
ATOM FIGH CG GLU 670	40 == 30.509 1 00 45
Amore CD GLU 670	14.819 30.243 1.00
3186 OE1 Otto	13.345 30.070 1 00 75
ATUM 5187 OE2 CITY	50.512 12.552 20.202 51.35
ATOM 5188 C	48.458 12.975 30 700 50.99
ATOM 5300	48 9/10
ATOM 5100 5	49 174 20.320 1.00 45 63
ATOM 5100 ALA 671	49 546 15 28.340 1.00 44 75
CA ALA 671	13.962 27.482 1.00
111011 5193 CB ALA 671	16.406 26.531 1 00
ATOM 5194 C ATA 4-	15.203 25 25
5195 O NY 3	49.931 17.313 25 405 43.27
ATOM 5106	50.485 18 3EE 0- 47.85
ATOM 5100 672	48.748 16.930 25.150 1.00 47.61
ATOM CA LEU 672	48 010 25.018 1.00 51 40
ATOM 5000 CB LEU 672	27.65/ 23.990 1.00
7701 5200 CG LEU 672	16.705 23.346 1 00 77
ATOM 5201 CD1 1.FIT C72	17.113 22.105 1 00 5
ATOM 5202 CD2 1711	47.114 17.425 20 020 1.00 58.92
ATOM 5203 C	45.269 15 977 23 2.00 58.60
ATOM 5204 6	47 315 21./53 1.00 60 33
ATOM 5205 120 6/2	47 200 24.514 1.00 55 01
ATOM 500	46 792 23.837 1.00 55 72
770 CA PHE 673	18.846 25.730 1 00
ATOM 5208 CB PHE 673	19.977 26 242
ATOM 5200 ~~	44.873 19.484 37.100 60.07
ATOM 5210 CD1	43.876 19.742 27.127 1.00 57.08
ATOM FOR	43 101 20.290 1.00 56 30
ATOM 500 PHE 673	43 632 26.813 1.00 57 67
A10M 5212 CE1 PHE 673	19.116 24.970 1 00
ATOM 5213 CE2 PHE 673	42.281 16.939 36 336
ATOM 5214 CD - 573	42.724 18.410 24 123
ATOM 5215 C 700	42.049 17 317 24.183 1.00 55.91
	46 974 23 24.720 1.00 56 42
SSSDIEELAS	46.974 20.854 27.238 1.00 63.00
SSSD/55145. v01	03.00
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MOTA	5216	0	PHE	<b>67</b> 3	46.926	22.085	27.155	1.00	65.31
ATOM	5217	N	ASP	674	47.786	20.223	28.081	1.00	64.08
MOTA	5219	CA	ASP	674	48.656	20.954	28.999	1.00	64.97
ATOM	5220	CB	ASP	674	48.545	20.375	30.409	1.00	<b>65.1</b> 3
ATOM	5221	CG	ASP	674	47.128	20.358	30.923	1.00	67.33
ATOM	5222	OD1	ASP	674	46.684	19.283	31.372	1.00	66.68
MOTA	5223	OD2	ASP	674	46.462	21.416	30.869	1.00	69.20
MOTA	5224	C	ASP	674	50.132	20.971	28.603	1.00	66.38
MOTA	5225	0	ASP	674	50.984	21.304	29.434	1.00	68.44
MOTA	5226	N	ARG	675	50.441	20.585	27.365	1.00	65.68
ATOM	5228	CA	ARG	675	51.829	20.550	26.883	1.00	63.71
MOTA	5229	CB	ARG	675	52.321	21.970	26.576	1.00	63.67
ATOM	5230	CG	ARG	675	51.491	22.685	25.531	1.00	67.65
MOTA	5231	CD	ARG	675	52.094	24.034	25.146	1.00	73.20
MOTA	5232	NE	ARG	675	53.382	23.911	24.457	1.00	74.09
MOTA	5234	CZ	ARG	675	54.159	24.939	24.122	1.00	73.41
ATOM	5235	NHl	ARG	675	53.788	26.182	24.408	1.00	72.90
MOTA	5238	NH2	ARG	675	55.324	24.720	23.524	1.00	71.96
ATOM	5241	С	ARG	675	52.780	19.864	27.876	1.00	61.41
ATOM	5242	0	ARG	675	53.960	20.208	27.966	1.00	62.62
ATOM	5243	N	ILE	676	52.248	18.903	28.627	1.00	59.15
MOTA	5245	CA	ILE	676	53.016	18.162	29.623	1.00	56.88
MOTA	5246	CB	ILE	676	52.175	17.904	30.891	1.00	56.26
ATOM	5247	CG2	ILE	675	52.871	16.904	31.807	1.00	53.11
ATOM	5248	CG1	ILE	676	51.920	19.224	31.614	1 00	57.86
ATOM	5249	CD1	ILE	676	51.038	19.096	32.835	1.00	61.05
ATOM	5250	C	ILE	676	53.494	16.828	29.070	1.00	56.58
MOTA	5251	0	ILE	676	52.727	15.869	28.985	1.00	58.12
ATOM	5252	N	TYR	677	54.760	16.773	28.680	1.00	54.34
MOTA	5254	C'A	TYR	677	55.340	15.556	28.143	1.00	51.14
ATOM	5255	CB	TYR	677	56.240	15.868	26.954	1.00	52.37
ATOM	5256	CG	TYR	677	55.488	16.315	25.719	1.00	56.21
MOTA	5257	CD1	TYR	677	55.187	17.660	25.512	1.00	56.78
MOTA	5258	CE1	TYR	677	54.534	18.086	24.353	1.00	57.54
MOTA	5259	CD2	TYR	677	55.113	15.395	24.738	1.00	57.82
ATOM	5260	CE2	TYR	677	54.458	15.809	23.571	1.00	59.32
MOTA	5261	CZ	TYR	677	54.177	17.159	23.385	1.00	59.59
MOTA	5262	OH	TYR	677	53.557	17.589	22.230	1.00	60.15
MOTA	5264	С	TYR	677	56.124	14.854	29.224	1.00	48.64
ATOM	5265	0	TYR	677	57.040	15.430	29.812	1.00	50.45
ATOM	5266	N	THR	678	55.733	13.621	29.510	1.00	44.59
MOTA	5268	CA	THR	678	56.397	12.834	30.524	1.00	42.21
MOTA	5269	CB	THR	678	55.524	12.726	31.791	1.00	43.55
MOTA	5270	OG1	THR	678	54.302	12.045	31.475	1.00	47.42
MOTA	5272	CG2	THR	678	55.190	14.105	32.327	1.00	48.74
MOTA	5273	С	THR	678	56.634	11.432	29.992	1.00	39.94
ATOM	5274	0	THR	678	56.207	11.085	28.892	1.00	39.34
MOTA	5275	N	HIS	679	57.312	10.616	30.784	1.00	38.54
MOTA	5277	CA	HIS	679	57.532	9.248	30.390	1.00	38.29
ATOM	5278	CB	HIS	679	58.441	8.546	31.391	1.00	39.51
ATOM	5279	CG	HIS	679	59.869	8.997	31.331	1.00	43.13
ATOM	5280	CD2	HIS	679	60.630	9.668	32.233	1.00	43.49
ATOM	5281	ND1	HIS	679	60.694	8.726	30.263	1.00	43.00
ATOM	5283	CE1	HIS	679	61.903	9.201	30.510	1.00	43.62
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ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	5286 5287 5288 5290 5291 5292 5293 5294 5295 5298 5299 5300 5302 5303 5304 5306	G C C C C C C C C C C C C C C C C C C C	HIS GLN GLN GLN GLN GLN GLN SER SER SER SER	679 679 680 680	61.889 56.147 55.898 55.228 53.867 53.214 53.835 53.677 52.595 54.767 53.013 51.968 53.427 52.665 52.929 54.307 53.066	9.776 8.599 7.667 9.156 8.649 9.010 8.278 6.756 6.225 6.050 9.099 8.505 10.155 10.571 12.034 12.286 9.620	30.359 29.593 31.142 31.209 32.543 33.732 33.660 33.908 33.348 30.036 29.758 29.349 28.182 27.813 27.620	1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00	44.68 39.42 40.00 38.96 38.84 40.90 44.42 44.47 45.52 42.06 38.25 39.27 37.00 38.02 40.29 47.29
ATOM ATOM ATOM	5307 5308 5310	O N CA	SER ASP ASP	681 682	52.289 54.281	9.620 9.366 9.077	27.051 26.136 27.162	1.00 1.00 1.00	37.43 37.86
ATOM ATOM ATOM	5311 5312 5313	CB CG	ASP ASP	682 682 682	54.800 56.284 57.224	8.106 7.820 8.732	26.205 26.464	1.00 1.00	35.23 33.24 31.85
ATOM ATOM	5314 5315	OD1 OD2 C		682 682 682	58.445 56.763 54.015	8.537 9.620 6.810	25.677 25.826 24.908	1.00 1.00 1.00	34.18 31.79 29.15
MOTA	5316 5317	O N		682 683	53.788 53.653	6.087	25	1.00 1.00	31.52 31 93

A A A A A A A A. MOTA VAL 683 53.653 ATOM 5319 6.499 27.617 C'A VAL 1.00 683 33.14 52.879 MOTA 5.293 5320 27.935 CB VAL 1.00 683 32.79 52.725 ATOM 5.095 5321 29.478 CG1 VAL 1.00 34.56 683 51.653 ATOM 4.059 5322 29.790 CG2 1.00 VAL 683 32.39 54.050 ATOM 4.649 5323 30.088 С VAL 1.00 683 28.08 51.506 ATOM 5324 5.338 27.245 0 1.00 VAL 683 31.45 51.008 ATOM 4.311 5325 26.779 N 1.00 TRP 30.37 684 50.919 ATOM 6.531 5327 27.147 CA 1.00 TRP 31.04 684 49.638 ATOM 6.686 5328 26.464 CB TRP 1.00 31.23 684 49.158 ATOM 5329 8.137 26.525 CG 1.00 TRP 684 34.14 47.913 MOTA 5330 8.423 25.694 CD2 TRP 1.00 684 37.17 46.573 MOTA 8.593 5331 26.187 CE2 1.00 TRP 684 38.61 45.755 ATOM 8.888 5332 CE3 25.064 TRP 1.00 37.91 684 45.978 8.528 ATOM 5333 27.452 CD1 1.00 TRP 37.63 684 47.850 MOTA 8.612 24.337 5334 NE1 TRP 1.00 684 37.39 46.560 ATOM 5336 8.894 23.956 CZ2 1.00 TRP 34.76 684 44.380 9.118 ATOM 5337 25.181 CZ3 1.00 TRP 34.79 684 44.611 ATOM 8.759 5338 27.563 CH2 1.00 TRP 38.53 684 43.830 ATOM 9.048 26.428 5339 C TRP 1.00 684 37.59 49.876 ATOM 6.294 5340 25.013 0 1.00 TRP 29.99 684 49.254 ATOM 5.356 5341 24.503 N SER 1.00 30.82 685 50.815 ATOM 6.992 5343 24.380 CA SER 1.00 28.28 685 51.174 MOTA 6.738 5344 22.986 CB 1.00 SER 685 27.54 52.444 ATOM 7.504 5345 22.631 OG 1.00 SER 26.69 685 52.355 ATOM 8.874 5347 22.986 C SER 1.00 32.15 685 **51.39**9 MOTA 5.249 5348 22.737 0 SER 1.00 26.41 685 50.968 ATOM 4.709 21.713 5349 N PHE 1.00 686 29.52 52.065 4.582 23.676 1.00 26.47 SSSD/55145. v01

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MOTA	5351	CA	PHE	686	52.325	3.151	23.563	1.00	26.35
ATOM	5352	CB	PHE	686	53.167	2.668	24.754	1.00	25.01
MOTA	5353	CG	PHE	686	53.447	1.182	24.742	1.00	27.24
MOTA	5354	CD1	PHE	686	54.187	0.600	23.712	1.00	24.88
MOTA	5355	CD2	PHE	686	52.915	0.351	25.729	1.00	24.99
MOTA	5356	CE1	PHE	686	54.389	-0.783	23.655	1.00	22.77
MOTA	5357	CE2	PHE	686	53.113	-1.036	25.679	1.00	28.39
ATOM	5358	CZ	PHE	686	53.853	-1.601	24.631	1.00	22.71
ATOM	5359	С	PHE	686	50.997	2.366	23.466	1.00	28.82
ATOM	5360	0	PHE	686	50.892	1.398	22.696	1.00	26.41
ATOM	5361	N	GLY	687	49.988	2.797	24.229	1.00	29.65
MOTA	5363	CA	GLY	687	48.692	2.134	24.194	1.00	29.88
ATOM	5364	С	GLY	687	48.099	2.158	22.794	1.00	29.57
ATOM	5365	o	GLY	687	47.560	1.165	22.300	1.00	30.38
ATOM	5366	N	VAL	688	48.222	3.310	22.147	1.00	29.19
ATOM	5368	CA	VAL	688	47.718	3,478	20.795	1.00	25.09
ATOM	5369	CB	VAL	688	47.747	4.956	20.359	1.00	22.52
ATOM	5370	CG1	VAL	688	47.106	5.115	18.985	1.00	21.13
ATOM	5371	CG2	VAL	688	47.001	5.810	21.366	1.00	22.50
ATOM	5372	C	VAL	688	48.574	2.636	19.865	1.00	23.82
ATOM	5373	0	VAL	688	48.080	2.132	18.871	1.00	25.39
ATOM	5374	Ŋ	LEU	689	49.849	2.463	20.208	1.00	24.46
ATOM	5376	CA	LEU	689	50.764	1.655	19.401	1.00	25.68
ATOM	5377	C.B	LEU	689	52.222	1.893	19.834	1.00	25.93
MOTA	5379	CG	LEU	689	53.374	1.307	19.004	1.00	25.01
ATOM	5379	CD1	LEU	689	54.655	2.080	19.257	1.00	25.86
ATOM	5380	CD2	LEU	689	53.593	-0.145	19.318	1.00	24.90
ATOM	5381	C	LEU	689	50.374	0.171	19.531	1.00	26.50
ATOM	5382	Ó	LEU	689	50.464	-0.578	18.558	1.00	27.13
ATOM	5383	N	LEU	690	49.927	-0.234	20.724	1.00	27.76
MOTA	5385	CA	LEU	690	49.481	-1.610	20.980	1.00	28.59
ATOM	5386	CB	LEU	690	49.087	-1.800	22.447	1.00	30.38
ATOM	5387	CG	LEU	690	50.121	-2.065	23.545	1.00	29.57
ATOM	5388	CD1	LEU	690	49.435	-1.966	24.907	1.00	27.40
ATOM	5389	CD2	LEU	690	50.744	-3.431	23.360	1.00	28.79
ATOM	5390	С	LEU	690	48.242	-1.849	20.134	1.00	28.77
MOTA	5391	0	LEU	690	48.055	-2.922	19.573	1.00	28.07
ATOM	5392	N	TRP	691	47.383	-0.838	20.075	1.00	29.58
ATOM	5394	CA	TRP	691	46.166	-0.921	19.275	1.00	30.53
ATOM	5395	CB	TRP	691	45.327	0.349	19.451	1.00	28.28
ATOM	5396	CG	TRP	691	43.985	0.300	18.769	1.00	25.86
ATOM	5397	CD2	TRP	691	43.702	0.689	17.421	1.00	23.99
ATOM	5398	CE2	TRP	691	42.321	0.498	17.215	1.00	25.08
ATOM	5399	CE3	TRP	691	44.487	1.165	16.367	1.00	20.88
ATOM	5400	CD1	TRP	691	42.791	-0.090	19.314	1.00	23.72
MOTA	5401	NE1	TRP	691	41.786	0.031	18.389	1.00	26.15
ATOM	5403	CZ2	TRP	691	41.704	0.788	15.997	1.00	25.07
ATOM	5404	CZ3	TRP	691	43.883	1.448	15.163	1.00	22.80
ATOM	5405	CH2	TRP	691	42.501	1.251	14.982	1.00	24.95
ATOM	5406	C	TRP	691	46.566	-1.116	17.811	1.00	30.63
ATOM	5407	0	TRP	691	45.943	-1.892	17.093	1.00	33.02
ATOM	5408	N	GLU	692	47.625	-0.431	17.386	1.00	31.00
ATOM	5410	CA	GLU	692	48.130	-0.545	16.018	1.00	29.00
ATOM	5411	CB	GLU	692	49.285	0.426	15.778	1.00	26.55
						J. 120	23.770		20.55

ATO	OM 543	12 ~							
ATO					48.873		6 15.65	1 1.00	29.90
ATO					50.040		1 15.31		
ATO					50.770				
ATO					50.227	3.11			_
ATO			GL		48.622	-1.95			
ATO		_	GL		48.474	-2.46		_	
ATO		_	IL		49.258	-2.57			
			IL		49.766	-3.933			
ATO			IL	€ 693	50.634	-4.360			
ATO			2 IL	693	51.006	-5.845			32.36
ATO			l ILE	693	<b>51.90</b> 9	-3.506			34.39
ATO			ILE	693	52.696	-3.693			30.30
ATO		_	ILE	693	48.638	-4.939		1.00	25.66
ATO		5 0	ILE	693	48.633	-5.738		1.00	30.63
ATO		7 N	PHE	694	47.644	-4.858		1.00	31.10
ATOM	_	CA	PHE	694	46.543	-5.793		1.00	32.60
ATON		CB	PHE	694	45.938	-5.970		1.00	33.86
ATOM	4 5431	CG	PHE		46.941			1.00	35.66
ATOM	1 5432	CD1	PHE		47.460	-6.499	19.559	1.00	35.70
ATOM	1 5433	CD2	PHE	694	47.449	-5.684	20.556	1.00	37.18
ATOM	5434	CE1	PHE	694	48.473	-7.794	19.426	1.00	34.37
ATOM	5435	CE2	PHE	694	48.456	-6 150	21.392	1.00	36.90
ATOM	5436		PHE	694	48.970	-8.265	20.255	1.00	31.89
ATOM	5437	С	PHE	694	45.532	-7.446	21.234	1.00	34.95
ATOM	5438	O	PHE	694		-5.576	16.049	1.00	34.26
ATOM	5439	N	THR	695	44.702	-6.442	15.787	1.00	37.52
ATOM		CA	THR	695	45.636	-4.441	15.359	1.00	32.23
ATOM		CB	THR		44.775	-4.160	14.215	1.00	28.08
ATOM		OG1	THR	695 695	44.186	-2.728	14.241	1.00	25.71
ATOM	5445	CG2	THR	695	45.237	-1.762	14.228	1.00	24.94
ATOM	5446	С	THR	695	43.353	-2.528	15.468	1.00	23.07
ATOM	5447	ō	'THR	695	45.615	-4.348	12.955	1.00	27.53
ATOM	5448	N	LEU	696	45.166	-4.066	11.845	1.00	30.89
ATOM	5450	CA	LEU		46.833	-4.848	13.145	1.00	27.73
ATOM	5451	CB	LEU	696	47.781	-5.081	12.061	1.00	28.99
ATOM	5452	CG	LEU	696	47.370	-6.297	11.226	1.00	27.78
ATOM	5453	CD1	LEU	696	47.379	-7.591	12.047	1.00	29.89
ATOM	5454	CD2	LEU	696	47.251	-8.823	11.164	1.00	29.96
ATOM	5455	C	LEU	696	48.668	-7.656	12.803	1.00	30.20
ATOM	5456	0	LEU	696	48.044	-3.853	11.179	1.00	30.33
ATOM	5457	N	GLY	696	48.006	-3.926	9.948	1.00	29.41
ATOM	5459	CA		697	48.374	-2.738	11.831		30.92
ATOM	5460	C	GLY	697	48.655	-1.503	11.113		30.35
ATOM	5461	0	GLY	697	47.420	-0.650	10.912		30.65
ATOM	5462		GLY	697	47.359	0.178	10.000		30.01
ATOM	5464	N	GLY	698	46.428	-0.836			30.50
ATOM	5465	CA	GLY	698	45.209	-0.063			30.36
ATOM		C	GLY	698	45.416	1.415			30.07
ATOM	5466 5467	0.	GLY	698	46.320	1.809			30.56
ATOM	5467	N	SER	699	44.554	2.228			29.65
	5469	CA		699	44.597	3.674			
ATOM	5470	CB		699	44.263		_	_	28.42
ATOM	5471			699	43.960				24.61
ATOM	5473		SER	699	43.621			_	31.25
ATOM	5474	0	SER ·	699	42.406				8.27
SSSD/FF	• • • •			•				1.00 2	7.14

ATOM	5475	N	PRO	700	44.160	4.682	13.675	1.00	29.29
ATOM	5476	CD	PRO	700	45.587	4.867	13.999	1.00	26.09
MOTA	5477	CA	PRO	700	43.303	5.155	14.764	1.00	29.30
MOTA	5478	CB	PRO	700	44.319	5.624	15.812	1.00	27.68
MOTA	5479	CG	PRO	700	45.531	5.982	14.985	1.00	27.85
ATOM	5480	C	PRO	700	42.413	6.305	14.306	1.00	29.71
MOTA	5481	0	PRO	700	42.800	7.096	13.446	1.00	31.38
ATOM	5482	N	TYR	701	41.204	6.357	14.854	1.00	29.51
ATOM	5484	CA	TYR	701	40.246	7.419	14.548	1.00	30.25
MOTA	5485	CB	TYR	701	40.559	8.647	15.405	1.00	33.50
MOTA	5486	CG	TYR	701	40.321	8.413	16.866	1.00	37.84
ATOM	5487	CD1	TYR	701	41.323	8.638	17.803	1.00	40.05
MOTA	5488	CE1	TYR	701	41.092	8.412	19.158	1.00	42.28
MOTA	5489	CD2	TYR	701	39.084	7.965	17.310	1.00	41.54
MOTA	5490	CE2	TYR	701	38.845	7.738	18.653	1.00	43.70
MOTA	5491	CZ	TYR	701	39.845	7.963	19.574	1.00	42.63
MOTA	5492	OH	TYR	701	39.584	7.716	20.907	1.00	45.31
MOTA	5494	С	TYR	701	40.173	7.829	13.088	1.00	28.45
MOTA	5495	0	TYR	701	40.356	9.001	12.760	1.00	29.03
ATOM	5496	Ñ	PRO	702	39.901	6.867	12.191	1.00	28.05
ATOM	5497	CD	PRO	702	39.671	5.430	12.417	1.00	2690
ATOM	5498	CA	PRO	702	39.815	7.181	10.764	1.00	27.48
ATOM	5499	CB	PRO	702	39.610	5.807	10.119	1.00	2 <b>7.0</b> 6
ATOM	5500	CG	PRO	702	38.923	5.036	11.169	1.00	28.28
ATOM ATOM	5501 5502	C O	PRO	702	38.689	8.145	10.440	1.00	26.81
ATOM	5502 5503	N	PRO GLY	702 703	37.554	7.953	10.865	1.00	26.26
ATOM	5505	CA	GLY	703	39.035 38.085	9.192 <b>1</b> 0.217	9.693 9.295	1.00	28.48
ATOM	5506	C	GLY	703	37.862	11.285	10.351	1.00	26.54 28.03
ATOM	5507	0	GLY	703	37.110	12.231	10.108	1.00	28.93
ATOM	5508	N	VAL	704	38.518	11.149	11.505	1.00	28.16
ATOM	5510	CA	VAL	704	38.369	12.081	12.619	1.00	29.55
ATOM	5511	СВ	VAL	704	38.473	11.360	13.984	1.00	28.50
ATOM	5512	CG1	VAL	704	38.330	12.350	15.135	1.00	28.07
MOTA	5513	CG2	VAL	704	37.403	10.295	14.091	1.00	29.78
ATOM	5514	C	VAL	704	39.375	13.227	12.588	1.00	32.00
ATOM	5515	0	VAL	704	40.578	13.028	12.758	1.00	33.85
ATOM	5516	N	PRO	705	38.888	14.446	12.336	1.00	33.56
MOTA	5517	CD	PRO	705	37.512	14.763	11.906	1.00	33.69
ATOM	5518	CA	PRO	705	39.745	15.628	12.280	1.00	32.65
ATOM	5519	CB	PRO	705	38.863	16.647	11.569	1.00	34.10
ATOM	5520	CG	PRO	705	37.478	16.256	12.021	1.00	36.38
ATOM	5521	C	PRO	705	40.164	16.081	13.668	1.00	33.22
ATOM	5522	0	PRO	705	39.549	15.708	14.668	1.00	33.26
ATOM	5523	N	VAL	706	41.198	16.912	13.710	1.00	34.61
ATOM	5525	CA	VAL	706	41.764	17.417	14.954	1.00	37.72
ATOM	5526 5527	CB	VAL	706	42.803	18.527	14.673	1.00	39.14
ATOM ATOM	5527 5528	CG1 CG2	VAL VAL	706 706	43.483	18.941	15.957	1.00	39.12
ATOM	5529	C	VAL	706	43.836	18.038	13.670	1.00	41.07
MOTA	5530	0	VAL	706	40.740	17.934 17.536	15.969	1.00	38.70
ATOM	5530 5531	N	GLU	700	40.761 39.834	17.536	17.136	1.00	38.42
MOTA	5533	CA	GLU	707	38.823	18.796 19.375	15.517 16.395	1.00	40.43
ATOM	5534	CB	GLU	707	37.973	20.379	15.621	1.00	40.66 43.40
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	MOTA	5535	С	GLU	705							
	ATOM	5536	0	GLU	707	J,	. 940	18	3.316	7 000		
	ATOM	5537	N		707	37.	642			7.028	1.00	41.03
	MOTA	5539		GLU	708	37.	560			8.231	1.00	41.52
	ATOM	5540	CA	GLU.	708	36.	708			6.224	1.00	41.62
	ATOM	5541	CB	GLU	708	36	179	10	.243 1	6.700	1.00	41.06
		_	CG	GLU	708	35.	201		.425 1	5.523	1.00	45.19
		5542	CD	GLU	708	24	28I		.221 1	4.571	1.00	40.19
		5543	OE1	GLU	708	34.	063	16	825 1	5.258		48.74
	TOM	5544	OE2	GLU		33.	523	16.	203 16	5.207	_	57.18
A	TOM	5545	С		708	33.6	46		_		1.00	54.30
A		5546	0	GLU	708	37.4	43		_		1.00	51.76
A'	<b>-</b>	5547		GLU	708	36.8	67	14		.694		38.39
		54.9	N	LEU	709	38.7	25	14.		.696		86.76
	<b>n</b>		CA	LEU	709	39.5	E E	15.		.434		7.78
		550	CB	LEU	709	41.0	22	14.	327 18	30.		7.78
	rom 5	551	CG		709	41.0	07	14.	255 17			8.13
	OM 5	552				41.9	84	13.9		_		5.45
	OM 5		~~ -		709	41.82	25	12.0				5.57
AT			_ '		709	43.40	7.	13.9			.00 3	2.33
AT			_		709	39.55	o.	14.0		484 1	.00 3	1.98
ATO		· <b>-</b> - `		LEU 7	709	39.36	3	14.9		716 1	.00 38	3.31
ATO		556 1	1 E	PHE 7	10	39.77		14.2		717 1		3.16
			:A p	HE 7	10	39.77		16.2	54 19.			7.16
ATO			В р		10	39.80		16.9	73 21.			.09
ATC		_			10	39.99	7	18.4	<sup>75</sup> 20.			.61
ATC		61 C	_			41.32	8 ;	18.83	34 20.			.22
ATO	M 55				10	42.39	5 ;	17.93			00 51	. 7.7
ATO	M 556				10	41.513		20.07			00 52	. 94
ATO					LO	43.632					00 53	. 99
ATO			E2 PF	IE 71	LO	42.746		8.27	_	79 1.		
ATO			Z PF	IE 71	.0	43.807		0.42	? 19.0	21 1.	2 - 4	
	50	~	PH			20.507		9.51	<sup>7</sup> 19.0			
ATOM		7 0	PH			38.519	1	6.72	5 21.7		-	
ATOM		8 N	LY	_		38.539		6.424				35
ATOM		O CA				37.399		5.804				
ATOM						36.095	.16	5.587				68
ATOM	5572		LY:	- · <del>-</del> ·		34.977	16	.878		_		47
ATOM			LY		L	33.601	16	.765			0 44.	
ATOM			LYS	711	l	32.510	1.0				0 47.6	3
ATOM			LYS	711		31.158	1/	.206		2 1.0		
			LYS	711		30.030	16	- 873	20.96	0 1.0		
ATOM	5579	~	LYS			30.038	17	.412	20.15	0 1.00		
ATOM	5580	0	LYS			35.986	15	.173	22.26	-		
ATOM	5581	N	LEU		-	35.589	14	. 999	23.420			2
ATOM	5583	CA			3	6.392	14	.176		00		6
ATOM	5584		LEU		3	6.361	12	770	21.471			2
ATOM	5585	CB	LEU	712	3	6.922	11	210	21.898	1.00	42.5	
ATOM		CG	LEU	712	3	6.090	11.	843	20.809	1.00		
	5586	CD1	LEU	712	2	6.090	11.	528	19.560	1.00		
ATOM	5587	CD2	LEU	712	3	6.902	10.	620	18.636	1.00		
ATOM	5588	C	LEU			4.760	10.	868	19.951	_	36.28	
ATOM	5589	0		712	3.	7.158	12.	564	23.180		37.19	
ATOM	5590	N	LEU	712	36	5.697	11.	RRE	~~·TRO	1.00	42.34	
ATOM	5592		LEU	713	38	3.366	72 .	12-	24.107	1.00	40.77	
ATOM		CA	LEU	713	3 0	240	13.	-ZI	23.208	1.00	42.68	
_	5593	CB	LEU	713	40	.581	13.0	25	24.371	1.00	44 00	
3000	5594	CG	LEU	713	-3 U	· - 28T	13.7	10	24.100	1.00	44.05	
	5595	CD1	LEU	713	41	.418	13.1	14	22.963		45.45	
MOTA	5596	CD2	LEU		42	.676	13.9	45	22.750	1.00	44.78	
	5597	C		713		. 757	11.6		22 222	1.00	41.89	
	•		LEU	713		. 571	13.6		23.282	1.00	43.21	
SSSD/551	45 401						0	~ <del>4</del>	25.591	1.00	44.66	
	7.J. VIII											

	MOTA	5598	0	LEU	713	38.562	13.051	26.662	1.00	45.70	
	ATOM	5599	N	LYS	714	37.980	14.839	25.418	1.00	43.05	
	MOTA	5601	CA	LYS	714	37.300	15.510	26.524	1.00	42.19	
	ATOM	5602	CB	LYS	714	36.884	16.921	26.127	1.00	42.41	
	ATOM	5603	CG	LYS	714	38.076	17.828	25.918	1.00	46.10	
	ATOM	5604	CD	LYS	714	37.684	19.259	25.589	1.00	49.86	
	ATOM	5605	CE	LYS	714	38.939	20.097	25.292	1.00	52.55	
	ATOM	5606	NZ	LYS	714	39.889	20.148	26.459	1.00	50.17	
	ATOM	5610	С	LYS	714	36.104	14.728	27.054	1.00	42.39	
	MOTA	5611	0	LYS	714	35.767	14.824	28.237	1.00	43.44	
	MOTA	5612	N	GLU	715	35.480	13.934	26.192	1.00	40.44	
	MOTA	5614	CA	GLU	715	34.342	13.118	26.593	1.00	37.90	
٠	ATOM	5615	СВ	GLU	715	33.408	12.893	25.411	1.00	39.54	
	ATOM	5616	CG	GLU	715	32.800	14.174	24.846	1.00	45.20	
	ATOM	5617	CD	GLU	715	32.032	13.936	23.563	1.00	47.85	
	MOTA	5618	OE1	GLU	715	32.409	13.008	22.810	1.00	50.00	
	ATOM	5619	OE2	GLU	715	31.061	14.677	23.304	1.00	50.41	
	ATOM	5620	C	GLU	715	34.793	11.773	27.157	1.00	37.31	
	ATOM	5621	0	GLU	715	33.970	10.907	27.450	1.60	36.79	
	ATOM	5622	N	GLY	716	36.102	11.585	27.286	1.00	36.60	
	ATOM	5624	CA	GLY	716	36.623	10.336	27.819	1.00	37.11	
	MOTA	5625	C	GLY	716	36.503	9.140	26.887	1.00	38.30	
	ATOM	5626	0	GLY	716	36.603	7.994	27.34C	1.00	36.84	
	ATOM	5627	N	HIS	717	36.307	9.404	25.592	1.00	40.24	
	ATOM	5629	CA	HIS	717	36.167	8.353	24.579	1.00	42.63	
	ATOM	5630	СВ	HIS	717	35.800	8.951	23.217	1.00	43.11	
	ATOM	5631	CG	HIS	717	35.745	7.941	22.112	1.00	44.69	
	ATOM	5632	CD2	HIS	717	34.756	7.101	21.717	1.00	45.13	
	A.TOM	5633	ND1	HIS	717	36.818	7.683	21.283	1.00	47.31	
	MOTA	5635	CE1	HIS	717	36.494	6.728	20.425	1.00	47.61	
	ATOM	5636	NE2	HIS	717	35.250	6.357	20.670	1.00	44.95	
	MOTA	5638	C	HIS	717	37.451	7.567	24.413	1.00	44.84	
	MOTA	5639	0	HIS	717	38.528	8.152	24.295	1.00	46.79	
	MOTA	5640	N	ARG	718	37.313	6.247	24.337	1.00	45.44	
	ATOM	5642	CA	ARG	718	38.440	5.345	24.170	1.00	45.36	
	MOTA	5643	CB	ARG	718	38.614	4.496	25.434	1.00	43.82	
	MOTA	5644	CG	ARG	718	38.976	5.308	26.697	1.00	44.52	
	ATOM	5645	CD	ARG	718	40.284	6.065	26.476	1.00	45.02	
	ATOM	5646	NE	ARG	718	40.718	6.856	27.630	1.00	43.12	
	ATOM	5648	CZ	ARG	718	40.550	8.173	27.744	1.00	44.77	
	ATOM	5649	NH1	ARG	718	39.940	8.859	26.784	1.00	44.67	
	MOTA	5652	NH2	ARG	718	41.067	8.826	28.777	1.00	46.39	
	MOTA	5655	С	ARG	718	38.124	4.474	22.952	1.00	45.94	
	MOTA	<b>5</b> 656	0	ARG	718	36.953	4.243	22.645	1.00	47.59	
	ATOM	5657	N	MET	719	39.145	4.077	22.204	1.00	45.34	
	ATOM	5659	CA	MET	719	38.925	3.253	21.029	1.00	44.28	
	MOTA	5660	CB	MET	719	40.198	3.125	20.185	1.00	42.30	
	ATOM	5661	CG	MET	719	40.575	4.399	19.441	1.00	38.44	
	ATOM	5662	SD	MET	719	42.000	4.225	18.368	1.00	36.97	
	MOTA	5663	CE	MET	719	43.317	4.219	19.511	1.00	36.09	
	MOTA	5664	С	MET	719	38.415	1.877	21.418	1.00	46.21	
	ATOM	5665	0	MET	719	38.708	1.393	22.517	1.00	43.29	
	ATOM	5666	N	ASP	720	37.659	1.267	20.498	1.00	48.79	
	MOTA	5668	CA	ASP	720	37.069	-0.063	20.666	1.00	48.87	•
										,	

							2	78				
	ATOM	5669	CB	ASP	720							
	ATOM	5670	CG	ASP	720	36	.099	- (	.369	19.513	1.00	
	ATOM	5671	OD1	ASP		34	. 766		374	19.632		
	ATOM	5672	OD2	ASP	720	34	.762		.583	19.981		
	ATOM	5673	C		720 720	33	. 716		.259	19.354	-	•
		5674	0				.126		.154	20.688		58.64
		5675	N		720 721	39.	213		.992	20.125		46.10
		5677	CA		721 721	37.	788		. 272	21.322	1.00	44.13
	MOTA	5678	CB		721	38.	689		413	21.404	1.00	45.27
		679	CG		721	38.	172		436	22.416	1.00	43.25
		680	CD	•	21	39.	072			22.557	1.00	42.02
	TOM 5	681	CE	• • • •	21	38.	<b>60</b> 2			23.666	1.00	46.57
		682	AT D	• • • •	21	38.	300	-7.	_	23.141	1.00	49.96
	rom 5		_	<b>.</b>	21 21	37.9	937	8.	_	24.240	1.00	51.80
A	rom 5	687	_		21	38.7	769	-4.		20.031	1.00	56.08
		588 j				37.7	'36	-4.3		19.394	1.00	43.67
		589 (			22	39.9	95	-4.2		9.513	1.00	44.02
	'OM 56	590 (		PRO 72	22	41.2	81	-3.7		0.001	1.00	43.94
AT	OM 56					40.1		- 4 . 8		9.198	1.00	45.90
AT		92 0				41.6	65	-4.7		7.941	1.00	43.96
AT		93 c	_	_		42.0	46	-3.5		8.715	1.00	43.11
AT		ن 94		_ · <b>-</b>		39.7	72 .	-6.3		_	1.00	45.16
ATO		95 N		_		39.76	54.	6.8		_	1.00	43.09
ATO		97 C	_	ER 72. ER 72:		39.38	32	6.90		_		41.32
ATC						39.04	4 .	9.31				15.79
ATO		99 00				38.30	3 -	8.66		_		16.67
ATO		)1 C	SE			39.13	1 -	8.41		_		4.69
ATO		)2 <sub>(</sub>	SE			40.42	2	৪.96				9.79
ATO			AS			41.36	0 -	9.41	1 16			6.90
ATO	0					40.540		0.13	1 17	_		8.81
ATO		6 CB		_		41.826		08.0	4 .17	_		9.28
ATON	-					42.480		94	7 . 16.			2.10
ATOM		OD:		_		41.774		. 95	7 15.	F 0 0		5.86
ATOM						41.686		.140	) 15.	_		3.72
ATOM		, C	ASN			41.258		.503	14.		_	2.28
ATOM			ASN			42.665		. 931	18.			. 56
ATOM			CYS			43.621		. 274	18.	_		. 97
ATOM		CA	CYS			42.202		.859	20.		_	. 85
ATOM		CB	CYS	725	,	12.853		. 094	21.			.02
ATOM	5718	SG	CYS	725		12.708		. 583	20.1	311 1.		.18
ATOM	5719	C	CYS	725	4	3.424		577	22.5			. 75
ATOM		0	CYS	725	4	2.131	~9.	507	22.3	315 1.6		
ATOM	5721	N	THR	726		0.916	-9.	371	22.4	17 1.0		
ATOM	5723	CA	THR	726	4	2.866	-10.	880	23.2	49 1.0		
ATOM	5724	CB	THR	726	4	2.262	-10.	541	24.4	90 1.0		
ATOM	5725	OG1	THR	726	4.	3.251	-11.	444	25.2	91 1.0		
ATOM	5727	CG2	THR	726	4.	4.236	-10.	648	25.9	76 1.0		
ATOM	5728	С	THR		4.	3.982	-12.:	363	24.3			
ATOM	5729	0	THR	726 726	4.	1.788	-9.3	369	25.3			
ATOM	5730	N	ASN		42	3.305	-8.2	256	25.24	_	-	
ATOM	5732	CA	ASN	727	40	.829	-9.6	22	26.24			
ATOM	5733	CB	ASN	727	40	.335	-8.5	77	27.14			
ATOM	5734	CG	ASN	727	39	.190	-9.0	99	28.01		1	
ATOM	5735	OD1	ASN	727	39	.533	-10.4	09	28.71			7
			-2014	727	40	.709	-10.7	86	28.83			
SSSD/551	145. v01								UJ	3 1.00	70.4	3

68.43 **ATOM** 5736 ND2 ASN 727 38.500 -11.122 29.175 1.00 MOTA С ASN 5739 727 41.491 -8.091 28.023 1.00 50.29 **ATOM** 5740 0 ASN 727 41.467 -6.976 28.540 1.00 49.88 MOTA 5741 N GLU 728 -8.927 42.518 28.163 1.00 50.60 43.700 MOTA 5743 CA GLU 728 -8.597 28.956 1.00 49.33 MOTA 5744 -9.859 CB GLU 728 44.529 29.220 1.00 50.44 MOTA 5745 CG GLU 728 45.802 -9.600 30.008 1.00 55.30 ATOM 5746 CD GLU 46.577 728 -10.862 30.354 1.00 57.40 MOTA 5747 OE1 GLU 728 46.716 -11.754 29.489 1.00 56.75 728 MOTA 5748 OE2 GLU 47.062 -10.950 31.502 1.00 59.85 MOTA 5749 C GLU 728 44.539 -7.552 28.212 1.00 47.08 MOTA 5750 0 GLU 728 44.888 -6.512 28.776 1.00 48.02 MOTA 5751 N LEU 729 44.846 -7.821 26.945 1.00 43.34 MOTA 5753 LEU CA 729 45.630 -6.891 26.129 1.00 42.01 MOTA 5754 CB LEU 729 45.899 -7.500 24.751 1.00 39.46 ATOM 5755 CG LEU 729 -8.639 24.772 46.911 1.00 40.31 MOTA 5756 CD1 LEU 729 46.782 -9.482 23.531 1.00 42.21 MOTA 5757 CD2 LEU 729 -8.068 24.900 48.314 1.00 42.49 ATOM 5758 С LEU 729 44.901 -5.557 25.980 1.00 40.61 MOTA 5759 0 LEU 729 45.510 -4.481 25.953 1.00 38.33 MOTA 5760 N TYR 730 43.580 -5.637 25.909 1.00 39.07 ATOM 5762 CA TYR 730 25.773 42.761 -4.455 1.00 38.61 ATOM 5763 CB TYR 730 41.341 -4.837 25.369 1.00 36.79 MOTA 5764 CG TYR 730 40.454 -3.646 25.125 1.00 37.08 MOTA 5765 CD1 TYR 730 -2.721 32.86 40.760 24.127 1.00 ATOM 5766 CE1 TYR 730 23.912 39.961 1.00 -1.616 29.79 MOTA 5767 TYR CD2 730 39.328 -3.420 25.916 1.00 36.99 MOTA 5768 CE2 TYR 730 38.522 -2.312 25.704 1.00 36.69 MOTA 5769 CZ TYR 730 38.853 -1.412 24.706 1.00 32.69 MOTA 5770 TYR OH 730 38.044 -0.320 24.492 1.00 38.80 MOTA 5772 -3.662 С TYR 730 42.767 27.080 1.00 39.75 -2.430 MOTA 5773 0 TYR 730 42.781 27.065 1.00 40.53 731 MOTA 5774 N MET -4.360 42.738 28.210 1.00 41.88 ATOM 5776 CA MET 731 42.778 -3.684 29.509 1.00 45.34 **ATOM** 5777 CB MET 731 42.658 -4.697 30.646 1.00 53.46 MOTA 5778 CG MET 731 41.253 -5.248 30.836 1.00 64.30 MOTA 5779 SD MET 731 40.134 -4.095 31.653 1.00 75.78 MOTA 5780 CE MET 731 40.657 33.370 1.00 -4.338 69.70 MOTA 5781 MET 731 С 44.099 -2.927 29.614 1.00 41.53 MOTA 5782 0 MET 731 44.157 -1.814 30.138 1.00 37.91 ATOM 5783 N MET 732 45.156 -3.545 29.098 1.00 40.48 ATOM 5785 MET 732 CA 46.478 -2.937 29.091 1.00 40.23 ATOM 5786 MET CB 732 47.508 -3.872 28.436 1.00 40.29 MOTA 5787 CG MET 732 48.929 -3.307 28.390 1.00 38.07 MOTA SD 5788 MET 732 50.171 -4.522 27.908 1.00 37.65 MOTA 5789 CE MET 732 50.407 -5.343 29.431 1.00 37.90 MOTA 5790 C MET 732 46.378 -1.623 28.317 1.00 38.96 **ATOM** 5791 0 MET 732 46.843 -0.591 28.790 1.00 41.36 5792 **ATOM** MET 733 N 45.744 -1.663 27.148 1.00 36.94 MOTA 5794 CA MET 733 45.574 -0.463 26.340 1.00 35.19 MOTA 5795 44.796 CB MET 733 -0.769 25.070 1.00 36.07 **ATOM** 5796 CG MET 733 45.549 -1.577 24.048 1.00 35.99 ATOM MET 5797 SD 733 44.471 -1.851 22.641 1.00 40.05 MOTA 5798 CE MET 733 45.244 -3.351 21.909 1.00 33.13

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							2	80				
	MOTA	5799	C	MET	700							
7		5800	o		733	44	.800	(	0.560	27 24-		
A		5801	N	MET	733	45.	.207		L.719	27.141	1.00	37.29
A		803		ARG	734	43.	690			27.245	1.00	39.14
	_	804	CA	ARG	734	42.	849			27.735	1.00	38.76
	<b>.</b>		CB	ARG	734		577			28.532	1.00	39.49
		805	CG	ARG	734				.297	28.993	1.00	
		806	CD	ARG	734		699	- 0		27.856	1.00	40.33
		807	NE	ARG	734	40.	256	0		26.909		38.02
A	FOM 51	809	CZ	ARG		39.4	443			7.567	1.00	42.72
ΑT	OM 58	310	NH1	ARG	734	38.3	120		_		1.00	48.85
ΑT	'OM 58	313	NH2		734	37.4	135			7.700	1.00	52.35
AT	<b>.</b>		C	ARG	734	37.4				7.222	1.00	54.79
AT	-			ARG	734	43.6				8.338	1.00	54.69
AT			0	ARG	734	43.4			587 2	9.715	1.00	38.70
ATO			Ŋ	3	735				757 3	0.068	1.00	
			CA	<b></b>	735	44.5			782 30		1.00	40.92
ATO		21 (	75		735	45.3	79	1.:	208 31			38.76
ATC		22 (				46.32	25			_	1.00	38.60
ATC	M 582				735	45.62	22	-1.0		_	1.00	41.34
ATO					735	46.04	18	-2.1			1.00	44.66
ATO		_	-		35	44.65		-9.7		428		43.15
ATO			-	ASP 7	35	46.21	5			.313 1	.00	14.46
ATO			•	SP 7	35	46.23		2.3		.938 <u>1</u>		37.76
ATOM	_		С	YS 7	36	46.89	2	3.4				36.35
ATON			₹ C	YS 7	36	47 72	0	2.1				
			3 C	***	36	47.73		3.19	96 29.			5.39
ATOM		l so	_		36	48.379	9	2.65	52 27.			4.77
ATOM		. C		-		49.453	3	1.26		100 .		0.62
ATOM		0	C.			46.938	3	4.42		014		0.96
MOTA						47.516	;	5.49		<b>.</b>	00 3	5.98
ATOM	5836		TF			45.620		4.29	- •	_	00 3.	7.38
ATOM	5837		TR		7	44.772		5.42			00 38	3.50
ATOM	5838		TR		7	43.791				370 l.		16
ATOM		CG	TR	P 73	7	44.453		5.02		271 1.		.41
ATOM	5839	CD2		P 73	7	43.893		1.586		11 1.		.33
ATOM	5840	CEZ		P 735	7	44 050	3	3.718	3 25.0	20 1.		
	5841	CE3	TR			44.852	3	.583	23.9	92 1.0		.64
ATOM	5842	CD1			_	42.672	3	.040	24.9			.97
ATOM	5843	NE1		,		45.695	4	. 932	25.5			. 06
MOTA	5845	CZ2	TRE		-	45.941		. 336		-		. 56
MOTA	5846	CZ3			7	44.627		. 795		_		61
ATOM	5847	CH2	TRP			12.452		. 261	0.		0 38.	
ATOM	5848		TRP			3.426			23.77	-	0 38.	
ATOM	5849	C	TRP	737		4.028	~	. 145	22.77		0 38.	
ATOM		O	TRP	737		2.979		029	29.56	3 1.00		
	5850	N	HIS	738	4	4.575		658	29.39	8 1.00		
ATOM	5852	CA	HIS	738	- 4	4.575	5.	873	30.76	3 1.00		15
	5853	CB	HIS		4	3.932	6.	423	31.94	-		)1
	5854	CG	HIS	738	4	4.454		735	33.20	_	•	54
ATOM	5855	CD2		738	4.	3.742		154	24.45		2	20
3000.			HIS	738	43	3.473		379	34.45			5
3		ND1	HIS	738	43	3.220	· · ·	244	34.963		49.0	
3		CE1	HIS	738	42	2.659	J.,	.44	35.355		49.9	
		NE2	HIS	738	42	.798	5.8		36.357	1.00	52.9	- ว
3		C	HIS	738	. 32	178	7.1		36.146	1.00		
		C	HIS	738	44	.174	7.9	21	32.037	1.00	46.9	
ATOM 5	863 1	4	ALA		45	.314	8.3	56	32.021		45.26	
			ALA	739	43	.099	8.6		32.224		45.31	Ĺ
	•			739	43	.155	10.1	50		1.00	46.61	
		-~	ALA	739	41.		10.6		32.322	1.00	48.49	
SSSD/5514	5 v01						~ ~ . 0	- T	32.790	1.00	49.69	
1 7	~. VU I											

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ATOM	5867	C	ALA	739	44.272	10.682	33.224	1.00	50.77
MOTA	5868	0	ALA	739	45.004	11.601	32.846	1.00	51.77
ATOM	5869	N	VAL	740	44.336	10.138	34.439	1.00	51.47
ATOM	5871	CA	VAL	740	45.352	10.485	35.439	1.00	51.09
ATOM	5872	CB	VAL	740	44.897	10.075	36.850	1.00	52.40
ATOM	5873	CG1	VAL	740	45.847	10.624	37.878	1.00	53.38
MOTA	5874	CG2	VAL	740	43.485	10.544	37.105	1.00	55.18
ATOM	5875	С	VAL	740	46.649	9.727	35.130	1.00	48.99
ATOM	5876	0	VAL	740	46.773	8.534	35.440	1.00	47.72
MOTA	5877	N	PRO	741	47.646	10.421	34.565	1.00	48.31
MOTA	5878	CD	PRO	741	47.603	11.861	34.253	1.00	47.84
ATOM	5879	CA	PRO	741	48.949	9.852	34.197	1.00	48.51
MOTA	5880	CB	PRO	741	49.762	11.087	33.828	1.00	46.83
MOTA	5881	CG	PRO	741	48.714	1.2.000	33.255	1.00	46.21
ATOM	5882	C	PRO	741	49.641	9.016	35.275	1.00	49.12
ATOM	5883	O	PRO	741	50.449	8.139	34.955	1.00	46.57
ATOM	5884	N	SER	742	49.327	9.290	36.541	1.00	49.47
ATOM	5886	CA	SER	742	49.928	8.557	37.651	1.00	49.50
ATOM	5887	CB	SER	742	49.760	9.326	38.963	1.00	51.06
ATOM	5888	OG	SER	742	48.403	9.638	39.209	1.00	53.81
ATOM	5890	C	SER	742	49.339	7.159	37.787	1.00	48.81
ATOM	5891	0	SER	742	49.926	6.284	38.427	1.00	49.45
ATOM ATOM	5892	N	GLN	743	48.164	6.959	37.203	1.00	47.82
ATOM	5894 5895	CA CB	GLN GLN	743 743	47.529	5.658	37.273	1.00	46.34
ATOM	5896	CG	GLN	743. 743	46.022	5.791	37.432	1.00	49.74
ATOM	5897	CD	GLN	743	45.519 46 178	5.305	38.784	1.00	55.41
ATOM	5898	OE1	GLN	743	46.905	5.030	39.947	1.00	59.15
ATOM	5899	NE2	GLN	743	45.922	5.425 7.338	40.748	1.00	59.02
ATOM	5902	C	GLN	743	47.874	4.768	40.052 36.095	1.00	60.03 44.34
ATOM	5903	Ö	GLN	743	47.548	3.578	36.114	1.00	44.54
ATOM	5904	N	ARG	744	48.497	5.339	35.059	1.00	42.83
ATOM	5906	CA	ARG	744	48.914	4.559	33.880	1.00	40.34
ATOM	5907	CB	ARG	744	49.349	5.469	32.724	1.00	35.84
MOTA	5908	CG	ARG	744	48.296	6.406	32.190	1.00	28.25
ATOM	5909	CD	ARG	744	48.906	7.383	31.216	1.00	22.56
ATOM	5910	NE	ARG	744	47.948	8.437	30.922	1.00	28.09
ATOM	5912	CZ	ARG	744	48.258	9.658	30.493	1.00	32.83
ATOM	5913	NH1	ARG	744	49.524	10.001	30.278	1.00	34.44
ATOM	5916	NH2	ARG	744	47.307	10.569	30.360	1.00	32.00
ATOM	5919	C	ARG	744	50.110	3.712	34.295	1.00	41.58
MOTA	5920	0	ARG	744	50.906	4.124	35.145	1.00	45.48
ATOM	5921	N	PRO	745	50.223	2.489	33.754	1.00	40.97
ATOM	5922	CD	PRO	745	49.345	1.749	32.831	1.00	39.90
ATOM	5923	CA	PRO	745	51.381	1.685	34.157	1.00	39.77
ATOM	5924	CB	PRO	745	51.063	0.311	33.558	1.00	39.31
ATOM	5925	CG	PRO	745	50.255	0.642	32.344	1.00	40.98
MOTA	5926	C	PRO	745	52.664	2.269	33.573	1.00	38.44
ATOM	5927	0	PRO	745	52.631	3.009	32.595	1.00	39.64
MOTA	5928	N	THR	746	53.783	2.001	34.224	1.00	37.50
ATOM	5930	CA	THR	746	55.066	2.462	33.728	1.00	37.56
MOTA	5931	CB	THR	746	56.108	2.571	34.869	1.00	38.58
MOTA	5932	OG1	THR	746	56.286	1.285	35.487	1.00	43.28
ATOM	5934	CG2	THR	746	<b>5</b> 5. <b>6</b> 66	3.567	35.899	1.00	34.64

202	
ATOM 5935 C THR 746 55 546	
ATOM 5936 O mrs 33.546 1.393 32.730	
ATOM 5937 N DIE 33.118 0.234 32 817	
ATOM 5939 Ch NID 747 56.453 1.768 31.830 34.18	
ATOM 5940 CB 747 56.995 0.814 20.000 35.27	
ATOM 5941 747 58.025 1.425 30.080 1.00 33.48	
PHE 747 57 410 29.970 1.00 34 25	
Amore - 12 CD1 PHE 747 56 715 28.920 1.00 32.49	
3943 CD2 PHE 747 - 1.825 27.856 1 00 30	
3.749 29.018 1 00 22 a	
ATOM 5945 CE2 PHE 747 26.122 2.639 26.907 1.00 22.61	
ATOM 5946 CZ DV- 56.926 4.573 28.070 29.41	
ATOM 5947 C 56.223 4.014 37 015 1.00 32.93	
ATOM 5948 0 747 57.621 -0.363 31.50	
ATOM 5940 34.65	
ATOM 57-1 LYS 748 58 143 51.099 1.00 36 34	
ATOM 58 748 58 748 1.00 37 75	
5952 CB LYS 749 51.205 33.583 1.00 20 3	
5953 CG LYS 749 20.664 34.873 1.00 42	
ATOM 5954 CD LYS 748 53.958 -1.757 35.774 1 00	
AIOM 5955 OF THE SULL TO SULL	
ATOM 5956 NZ 130 61.183 -2.344 37 003	
ATOM 5960 C 170 -1.893 39 031	
ATOM 5961 0 -2.263 33 000 54.82	
ATION 57 48 57 202 - 33.882 1.00 39.65	
MON 552 N GLN 749 56 503 33.652 1.00 38 91	
ATOM - CA GLN 749 55 403 34.331 1.00 39.39	
70% 5965 CB GLN 749 54 177 22.742 34.623 1.00 40.70	
3966 CG GLN 740 1.991 35.140 1.00 42.22	
ATOM 5967 CD GLN 749 53 -1.149 36.373 1 00 50	
AIOM 5968 OEI GIN 750 -0.304 36 775	
ATOM 5969 NE2 CIV 53.272 0.914 36 885	
ATOM 5972 C 55.80	
ATOM 5973 0 55.009 -3.455 33 33: 1.00 60.05	
ATOM 5974 GLN 749 54.903 -4.670 33.334 1.00 40.03	
ATOM 54 P02 33.298 1.00 40 26	
ATOM CA LEU 750 54 400 32.278 1.00 39 18	
ATOM CB LEU 750 54 360 3.471 30.964 1.00 36.65	
3978 CG LEU 750 -2.039 29.927 1 00 3	
ATOM 5979 CD1 LET 750 -0.910 30.116 1.00 30	
ATOM 5980 CD2 LEU 750 0.210 29.125 1 00 31.52	
AIOM 5981 C Three 31.347 -1.435 29 935 -	
ATOM 5982 0 177 -4.255 30 477 1.00 31.37	
ATOM 5983 N 54.856 -5.267 39.963 35.81	
ATOM 5985 C7 56.626 -4.035 30.600 35.81	
ATOM 5006 751 57.607 5 000 30.820 1.00 37.38	
30.193 1.00 38 66	
751 60 075 30.411 1.00 35 42	
Nov. 5988 CG2 VAL 751 58 343 25.646 30.041 1.00 29 83	
3989 C VAI. 751 3.324 29.559 1 00 30 30	
ATOM 5990 O VAL 751 -6.314 30.974 1.00	
ATOM 5991 N CT 31 57.312 -7.401 30 306 41.63	
ATOM 5993 Ch 732 57.051 -6.174 32.267	
ATOM 5994 CD 56.766 -7.329 33 111	
ATOM 5005 CB GLU 752 56.674 -6.014 33.111 1.00 47.39	
MON 5095 CG GLU 752 57 950 5.514 34.587 1.00 50.66	
ATOM 5996 CD GLU 752 58 000 -6.243 35.101 1.00 54 77	
ATOM 5997 OE1 GLU 752 -6.101 36.612 1 00 55	
ATOM 5998 OE2 GLU 753 -4.972 37.102 1 00 5.14	
ATOM 5999 C GLU 752 -7.131 37.308 1 00 57	
55.496 -8.068 32.655 1.00	
SSSD/55145. v01	



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ATOM	6000	0	GLU	752	55.548	-9.261	32.328	1.00	46.25
MOTA	6001	N	ASP	753	54.380	-7.346	32.601	1.00	44.35
MOTA	6003	CA	ASP	753	53.099	-7.912	32.180	1.00	44.19
ATOM	6004	CB	ASP	753	52.059	-6.814	31.985	1.00	46.22
ATOM	6005	CG	ASP	753	51.512	-6.279	33.278	1.00	50.48
ATOM	6006	OD1	ASP	753	51.396	-7.062	34.248	1.00	52.15
MOTA	6007	OD2	ASP	<b>75</b> 3	51.170	-5.069	33.306	1.00	52.20
ATOM	6008	C	ASP	753	53.244	-8.608	30.849	1.00	44.54
ATOM	6009	0	ASP	753	52.770	-9.724	30.674	1.00	46.03
ATOM	6010	N	LEU	754	53.880	-7. <del>9</del> 18	29.906	1.00	44.43
ATOM	6012	CA	LEU	754	54.079	-8.438	28.563	1.00	43.70
ATOM	6013	CB	LEU	754	54.570	-7.339	27.618	1.00	43.48
MOTA	6014	CG	LEU	754	53.481	-6.350	27.201	1.00	44.67
ATOM	6015	CD1	LEU	754	54.095	-5.218	26.399	1.00	44.51
ATOM	601.6	CD2	LEU	754	52.384	-7.069	26.408	1.00	42.07
ATOM	6017	С	LEU	754	54.993	-9.642	28.512	1.00	43.14
MOTA	6018	0	LEU	754	<b>54.79</b> 5	-10.536	27.697	1.00	41.32
ATOM	6019	N	ASP	755	55.990	-9.671	29.383	1.00	44.74
MOTA	6021	CA	ASP	755	56.897	-10.800	29.426	1.00	47.24
ATOM	6022	CB	ASP	755	57.942	-10.575	30.517	1.00	51.26
ATOM	6023	CG	ASP	755	59.121	-11.518	30.407	1.00	55.39
MOTA	6024	OD1	ASP	755	59.739	-11.793	31.455	1.00	60.61
MOTA	6025	OD2	ASP	755	59.443	-11.970	29.283	1.00	57.16
ATOM	6026	C.	ASP	755	56.023	-12.005	29.771	1.00	47.67
ATOM	6027	0	ASP	755	56.041	-13.032	29.081	1.00	45.99
MOTA	6028	N	ARG	756	55.186	-11.816	30.789	1.00	46.72
MOTA	6030	CA	ARG	756	54.272	-12.851	31.256	1.00	46.25
ATOM	6031	CB	ARG	756	53.519	-12.368	32.499	1.00	46.31
ATOM	6032	CG	ARG	756	52.391	-13.297	32.953	1.00	46.99
ATOM	6033	CD	ARG	756	51.733	-12.776	34.227	1.00	48.10
ATOM	6034	NE	ARG	756	51.320	-11.379	34.118	1.00	53.67
ATOM	6036	CZ	ARG	756	50.294	-10.951	33.385	1.00	55.35
ATOM	6037	NHl	ARG	756	49.562	-11.812	32.684	1.00	54.10
ATOM	6040	NH2	ARG	756	50.008	-9.654	33.344	1.00	56.02
ATOM	6043	С	ARG	756	53.282	-13.261	30.175	1.00	45.05
ATOM	6044	0	ARG	756	53.213	-14.429	29.806	1.00	47.19
ATOM	6045	N	ILE	757	52.550	-12.289	29.647	1.00	43.47
ATOM	6047	CA	ILE	757	<b>51</b> . <b>55</b> 2	-12.553	28.617	1.00	43.80
MOTA	6048	CB	ILE	757	50.842	-11.241	28.161	1.00	42.02
ATOM	6049	CG2	ILE	757	49.811	-11.536	27.086	1.00	39.63
ATOM	6050	CG1	ILE	757	50.154	-10.578	29.361	1.00	40.00
ATOM	6051	CD1	ILE	757	49.600	-9.212	29.086	1.00	42.68
ATOM	6052	C	ILE	757	52.148	-13.296	27.428	1.00	46.03
ATOM	6053	0	ILE	757	51.549	-14.250	26.947	1.00	47.78
ATOM	6054	N	VAL	758	53.359	-12.925	27.015	1.00	49.03
ATOM	6056	CA	VAL	758	54.015	-13.584	25.884	1.00	51.51
ATOM	6057	CB	VAL	758	55.412	-12.971	25.556	1.00	50.75
ATOM	6058	CG1	VAL	758	56.105	-13.780	24.470	1.00	50.31
ATOM	6059	CG2	VAL	758	55.269	-11.541	25.081	1.00	52.52
ATOM	6060	C	VAL	758	54.209	-15.050	26.212	1.00	54.30
MOTA	6061	0	VAL	758	53.991	-15.915	25.369	1.00	54.80
ATOM	6062	N	ALA	759	54.617	-15.311	27.450	1.00	57.65
ATOM	6064	CA	ALA	759	54.858	-16.667	27.919	1.00	60.62
MOTA	6065	CB	ALA	759	55.423	-16.637	29.327	1.00	60.32

7.000		•	204
ATOM 6066 C	ALA 759	_	
ATOM 6067 O	_	53.571	-17.478 27.889 1.00
ATOM 6068 N	7 700	53.568	1.00 63 26
ATOM Come	LEU 760	52.475	26.25 47.478 1.00 65.01
ATOM COR-	LEU 760	51.191	28.305
ATOM COS	LEU 760	54.191	-17.533 28 333 1 aa
	LEU 760	50.302	-16.912 29 407 1 22
ATOM 6073 CD1		50.894	··16 962 30 - 1.00 65.66
ATOM 6074 CD2		49.988	716 246 27
ATOM 6075 C		51.109	1.00 64 77
ATOM 6076	LEU 760	50.483	31.227 1.00 66 67
ATOM COTT	LEU 760	49.390	17.335 26.984
24	THR 761	F1 100	-18.088 26.860 1 04.89
Amout CA .	THR 761	51.103	~16.933 25 073
710M 6080 CB 1		50.516	-16.882 24 4.00 65.24
ATOM 6001 000		50.829	21.034 1.00 64 44
ATOM 6002	THR 761	E 0 -	23.325 1.00 62 05
ATOM CO-	HR 761		44.463 24.660 1 a-
ATOM COO-	HR 761		-15.525 22 521 1 02.70
	HR 761	51.003	-18.044 23 760 · - · · · · · · · · · · · · · · · · ·
710M 6086 sc a	YS 1603	32.202	-18 201 22 - 1.00 64.71
5087 CG 10		18.536	-8 810 30 ± · · · · · · · 64 · 70
ATOM 6088 SD NO		69.178	20.295 0.50 23 07
ATOM GODO	224	CO	22.968 0.50 31 30
ATOM 6000 an	001	70	13.138 24.442 0 50 FR12
ATOM 2555	S 603	F ~	12.456 25.568 0 50 US PRT2
TOTAL OH2 TI		56.041	-7.885 16.319 0 34.22 PRT2
2685 OH2 mr.		/±./88	25 340 2 37.82 PRTS
2688 OH2 Tr		40.022	4.089 16 1.00 24.18
ATOM 2555		83.745	10.12/ 1.00 43 66
ATOM DOOL	3 4	0 2	1.00 27 20
ATOM 2007	· 3 5	7	7.482
ATOM 3700	3 6	0	6.505
- OH2 TTD	3 7	F1 A	.9.567 9.284 1 00
TION 2703 OH2 TIP	<b>5</b>	21.888 J	1.346 24 141 33.55
2/06 OH2 TTD	· ·	55.125	9.616 12 15 1.00 34.30
ATOM 2709 OH2 TTT		7.087	4.925 22 499 1.00 21.44
ATOM 2712 OH2 TT	3 10 5	2 145	1.00 20 70
ATOM 2215	3 11 4		13.180 1.00 21 14
ATOM 2710	12 4	C 00-	22.910 1 00
ATOM 3731	, 13 E		9.130 21.671
ATOM TIP3		~	2.335 28.803 1 00 37.09
Amous 2/24 OH2 TIP3	′	/·192 13	1.199 23 753
2727 Out man-	/:	9.201 17	295 30 1.00 32.96
ATOM 2730 OUR	16 82	2.988 11	500 38.51
ATOM 2733 OF 2	17 14	.096 -9	13.745 1.00 27 56
ATOM 2726	ם ג 18		0.333 1.00 23 53
ATOM DEED ON TIPS	19 26	- ·	5.313 1.00 43 15
ATOM 2745	20 3/	_	001 5.100 7 00
2/42 OH2 TTD3	~-	.305 -1.	615 16 900 .
2/45 ОН2 ТТРЗ	~-	.300 2	328 27 700 44.82
~/48 DW2 m===		.996 -11	502 30 1.00 45.23
ATOM 2751 OTTO	<sup>23</sup> 17.	261 -6.:	38.052 1.00 43 40
ATOM DEE.	44 on	70.	1.444 1.00 27 13
ATOM 2757	25 33		124 14.996 1 00
ATOM 2757 OH2 TIP3	· ·		294 6.872 1 22
2/60 OH2 TIP3	~ ~ ~ .		315 28 161 7 20
ATOM 2763 OH2 MTTS	<b>~</b> ~ ~ .	705 -17.1	92 13 260 49.20
ATOM 2766 OH2 TTP3	• • • • • • • • • • • • • • • • • • • •	639 13 q	15.269 1.00 30.16
ATOM 2769 ON2 TTT	<sup>!9</sup> -2.:	-0.5	7.092 1.00 41 04
ATOM 2772	0 34.9		76 11.086 1.00 44.00
ATOM 2775	1 80 7		69 19.070 1 00 34.89
ATOM 2775 OH2 TIP3 3	_ 00.1		65 9.324 1.00
	<sup>2</sup> 5.4	17 3.49	92 10 771
SSSD/55145. v01			10.771 1.00 34.07



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	13.542 1.00 30.81
	-10 718 4.889 11.542 1.00 51.35 ·
2778 OH2 11F3 33	29.486 -8.823 20.555 1.00 34.56
PMOM 2781 OH2 TIP3 34	6 151 3.065 13.021 2 00 48.13
2784 OH2 TIP3 35	31.907 2.919 0.361 1.00 30.12
2787 OH2 TIP3 36	19 974 1.928 -3.873 2 00 36.01
NTOM 2790 OH2 TIP3 37	61 976 2.660 32.604 1 00 20.12
- TOM 2793 OH2 TIP3 38	7 119 -3.759
- TON 2796 OH2 TIP3 39	-15 729 8.693 22.400 - 1 00 37.95
2799 OH2 TIP3 40	40 160 2.461 8.734 1.00 37.63
ATOM 2802 OH2 TIP3 41	10.248 11.349 0.190 1.00
2805 OH2 TIP3 42	25.056 9.143 17.185 1.00 57.03
2808 OH2 TIP3 43	19 150 18.734 1.00 37.19
7 TOM 2811 OH2 TIP3 44	17 144 3.98/ 1.00
NTOM 2814 OH2 TIP3 45	16 988 10.582 1.00
ATOM 2817 OH2 TIP3 46	7 073 14.829 1.00
NTOM 2820 OH2 TIP3 4/	5.510 1.00 24
ATOM 2823 OH2 TIP3 48	2 835 2.998 1.00
2826 OH2 TIP3 49	5 069 4.888 1.00
PMOM 2829 OH2 TIP3 50	5 517 24.999 1.00 22 69
ATOM 2832 OH2 TIP3 51	- 16 765 14·V/3
2835 OH2 TIP3 52	7 555 27.844 1.00
NTOM 2838 OH2 TIP3 53	1 595 6.080 1.00
NUM 2841 OH2 TIP3 54	12 084 25-108 1.00
2844 OH2 TIP3 55	68 239 6.953 16.647 1.00 29.47
2847 OH2 TIP3 56	73 621 20.852 18.820 1.00 22.31
2850 OH2 TIP3 5/	3 399 -3.294 -8.210 1.00 31.62
NTOM 2853 OH2 TIP3 56	37 999 10.824 5.505 1.00 40.76
ATOM 2856 OH2 TIP3 59	-9 515 -1.395 1.00
2859 OH2 TIP3 60	49 114 1.432 12.201 1.00 39.24
ATOM 2862 OH2 TIPS OF	41 257 4.012 29.003 2.00 34.36
ATOM 2865 OH2 TIP3 62	11 113 -12.848 1.250
ATOM 2868 OH2 TIP3 63	-1 221 -4.593 21.504 1.00 49.66
2871 OH2 TIPS 04	30 002 16.453 13.230 1 00 36.54
2874 OH2 TIP3 65	8.212 4.106 3.434 1.00 38.26
-mov 2877 OH2 TIP3 00	72.868 18.807 22.503 1.00 39.81
2880 OH2 TIP3 67	-8.056 -3.666 25.021 1.00 60.97
2083 OH2 TIP3 68	66 436 -4.683 28.000 1 00 42.25
2886 OH2 11F3 05	22.063 -20.641 4.804 -1.00 56.78
ATOM 2889 OH2 11P3 75	59.860 -7.407 4.035 - 1.00 59.32
2002 OH2 T1P3 /2	16 887 -13.832 -2.611 1.00 31.87
2895 OH2 TIPS	7.351 4.303 2.00 37.89
2898 OH2 11F3	32 901 2.922 13.865 1 00 39.12
ATOM 2901 OH2 11P3	- 0.173 -2.666 11.035 1.00 18.66
ATOM 2904 OH2 T1P3 /	17.533 2.317 5.808 1.00 29.04
-mom 2907 OH2 T1P3 /	27 183 3.730 6.345 2.00 30.53
7 TOM 2910 OH2 TIPS	5.887 9.703 ± 1 00 30.79
7 TOM 2913 OH2 TIPS	$\frac{1.614}{1.614}$ $\frac{-2.195}{1.614}$ $\frac{1.00}{1.00}$ $\frac{47.38}{1.00}$
ATOM 2916 OH2 TIPS	-5.304 -3.157 0.040 1.00 20.47
AMOM 2919 OH2 TIP3	17 401 2.918 1.373 - 1.00 24.44
rmom 2922 OH2 TIP3	3.188 3.159 1.00 21.11
ATOM 2925 OH2 TIP3	0.408 -2.516 22.270 1 00 17.62
NTOM 2928 OH2 TIP3	20.095 -6.123 -1.372 1.00 60.29
7 TOM 2931 OH2 TIP3	25 11.018 -15.627 7.421 1.00 39.47
ATOM 2934 OH2 TIP3	85 -12.037 11.797 1.00
ATOM 2937 OH2 TIP3	<b>60</b>
• • •	

ATOM 2940 OH2 TIP3	•
ATOM 2943 000	87 6.459 0.900
ATOM 2046 TIP3	88 -13.493 -3.278 1.00 30 71
ATOM 2546 OH2 TIP3	89 15 44 2 3 319 1 00
ATOM 2002 TIP3	90 2 -7.532 0.022 1 00
Amou 2952 OH2 TIP3	$\frac{-5.834}{21.29}$
ATOM 2955 OH2 TIPS of	4.833 -4.212 1.00 57.55
2958 OH2 TIP3 o	- 69.320 27 R12 1.00 44.52
ATOM 2961 OH2 TTD2	24.851 -12 973
ATOM 2964 Cura man-	4 60.303 0.285 1.00 44.73
ATOM 2967 OUR	5 10.488 - 33.927 1.00 40.13
ATOM 2072	b9 700 3.205 1.00 41 53
ATOM 2972 000	7 72 950 4.439 1.00 30 75
ATOM 2076 OH2 TIP3 98	3 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2
ATOM 2000	5.612 30.618 1 00
- One Tipe 10	1.007 11.717 1.00
2982 OH2 TID3 10	6.459 16 863
2985 OH2 TID2 10	20.70
ATOM 2988 OH2 TTP2 10	2 -13.529 7 860 12 1.00 47.13
ATOM 2991 OND TOTAL	26.795 -10.683 1.00 31.95
ATOM 2994 OU2 The	23.711 1 20.807 1.00 28.65
ATOM 2997 OTT	-2.187 12 22 18.309 1.00 28 20
ATOM 3000 OH2 T1P3 106	59.482 3.920 1.00 44.00
ATOM 3003 TIP3 107	3 3 5 4 5 7 5 7 5 7 5 7 5 7 5 7 5 7 5 7 5 7
ATOM 3006 TIP3 108	1.996
ATOM 1000 OH2 TIP3 109	25.00
ATO:: 3009 OH2 TIP3 110	1.477 25.476
3012 OH2 TIP3 111	15.594 14.349 1 00
3015 OH2 TIP3 113	2.396 -11.387 9.350 2.00 36.36
3018 OH2 TTP2 133	82.927 26.453 12.207 1.00 34.21
3021 OH2 TTD2 114	8.983 531 1.00 36.54
ATOM 3024 OH2 TIP3 17-	-8.690 4.367 1.00 47.01
ATOM 3027 OH2 TTP3 115	7.941 - 13.921 $3.504 - 1.00 - 41.25$
ATOM 3030 OV2	51.295 8.777 1.00 36 12
ATOM 3030	20 432 10.632 1.00 28 37
ATOM 2022 TIP3 118	72.882 - 13.637 1.00 31.33
ATOM 2074 TIP3 119	
ATOM 3040 TIP3 120	33.20 -11.863 22.711 1 00
ATOM 3042 OH2 TIP3 121	2.571 16 292 1 2
0H2 TIP3 122	7.160 1.00
- SU48 OH2 TIPS 122	3.827 -1 647
3051 OH2 TIP3 134	7.321
3054 OH2 TIP3 135	35.682 -1.725 0.534
3057 Otto men-	44 465 10 005 1 1.00 36.75
ATOM 30 3 +40	45.247 11.893 27 42
ATOM 3063 OV2	57.386 -10.506 -1.00 33.51
ATOM 300 1128	-3 032 14.020 1.00 45 70
ATOM 3069 000	85.621 13 10.644 1.00 38 40
ATOM 2072 1173 130	13.040 8.814 1.00 38 13
ATOM 3075 OHZ TIP3 131	2.760 2.176 1.00
ATOM 3075 OH2 TIP3 132	3.932 20.836 1 00
7 OH2 TIP3 133	7.467 -2.358 1 00
OH2 TID3 134	-9.967 n age 1 - 33.03
OH2 TIP3 125	13.716 -16.170 28.96
ATOM 3087 OH2 TIP2 135	-5.498 -3.706 16 170 - 44.64
ATOM 3090 OH2 TIPS 136	25.841 -12 949 1.00 43.17
ATOM 3093 000	16 285 3.950 1.00 41 14
ATOM 3096 OVE	86 457 6.585 1.00 45 75
ATOM 2000 OH2 TIP3 139	32 097 1.00 36 37
	44 936 2.044 2.224 1.00 30 35
SSSD/55145. v01	7.528 11 961
, vuj	1.00 46.60

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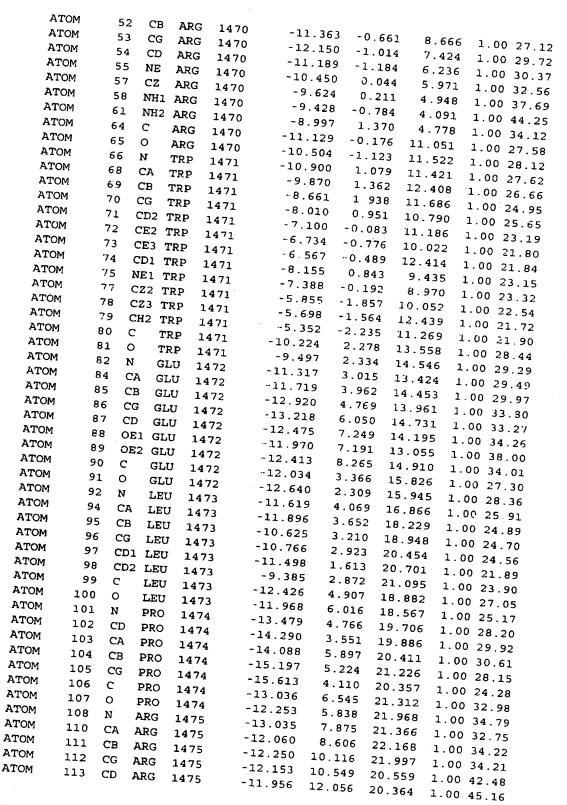
MOTA	3102	OH2	TIP3	141	80.781	12.162	16.353	1.00	41.46
ATOM	3105	OH2	TIP3	142	2.547	-7.532	-1.453	1.00	41.42
MOTA	3108	OH2	TIP3	143	31.850	-5.907	21.194	1.00	54.70
ATOM	3111	OH2	TIP3	144	74.524	-2.663	12.264	1.00	40.35
ATOM	3114	OH2	TIP3	145	7.592	6.769	-0.931	1.00	58.34
ATOM	3117	OH2	TIP3	146	71.168	5.735	21.648	1.00	27.86
ATOM	3120	OH2	TIP3		67.876	-4.900	8.725	1.00	33.58
ATOM	3123	OH2	TIP3		0.554	-10.181	6.605	1.00	75.65
ATOM	3126	OH2	TIP3	149	67.965	18.266	10.874	1.00	30.42
ATOM	3129	OH2	TIP3	150	3.509	8.125	4.021	1.00	40.77
MOTA	3132	OH2	TIP3	151	52.216	12.175	18.131	1.00	47.63
ATOM	3135	OH2	TIP3	152	-10.336	6.394	5.014	1.00	48.53
ATOM	3138	ОН2	TIP3	153	76.427	1.384	-1.196	1.00	47.21
ATOM	3141	OH2	TIP3		10.116	-12.199	17.089	1.00	70.16
ATOM	3144	OH2		155	34.043	14.595	18.314	1.00	40.56
AT'OM	3147	OH2	TIP3	156	2.488	-8.304	16.835	1.00	64.47
ATOM	3150	OH2	TIP3	157	29.610	1.954	6.685	1.00	48.74
ATOM	3153	OH2	TIP3	158	32.578	-17.270	12.109	1.00	37.35
ATOM	3156	OH2	TIP3	159	42.013	18.106	11.196	1.00	68.33
ATOM	3159	OH2	TIP3	160	87.646	10.346	5.465	1.00	75.39
ATOM	3162	OH2	TIP3	161	69.931	-3.739	24.921	1.00	70.42
ATOM	3165	OH2	TIP3	162	77.277	5.700	23.531	1.00	53.26
MOTA	3168	OH2	TIP3	163	34.172	15.704	1.865	1.00	44.88
ATOM	3171	OH2	TIP3	164	-9.871	7.514	7.751	1.00	39.18
ATOM	3174	OH2	TIP3	165	11.814	5.604	7.443	1.00	46.70
ATOM	3177	OH2	TIP3	166	-8.861	13.912	13.532	1.00	52.89
ATOM	3180	OH2	TIP3	167	32.195	3.409	18.336	1.00	32.33
MOTA	3183	OH2	TIP3	168	-8.858	9.696	24.279	1.00	38.90
ATOM	3186	OH2	TIP3	169	-1.135	-6.924	15.691	1.00	43.05
ATOM	3189	OH2	TIP3	170	79.806	0.323	15.371	1.00	36.91
MOTA	3192	OH2	TIP3	171	67.181	20.622	-1.545	1.00	44.72
MOTA	3195	OH2	TIP3	172	-0.823	3.732	1.065	1.00	52.11
ATOM	3198	OH2	TIP3	173	-0.130	6.021	2.491	1.00	40.87
ATOM	3201	OH2	TIP3	174	-1.027	8.941	1.064	1.00	60.72
ATOM	3204	OH2	TIP3	175	-5.566	8.867	2.163	1.00	47.25
ATOM	3207	OH2	TIP3	176	-7.259	10.294	4.033	1.00	53.61
ATOM	3210	OH2	TIP3	177	2.664	7.247	1.058	1.00	46 41
MOTA	3213	OH2	TIP3	178	5.295	10.728	8.257	1.00	39.84
ATOM	3216	OH2	TIP3	179	63.743	12.726	22.713	1.00	49.55
MOTA	3219	OH2	TIP3	180	79.165	1.016	17.948	1.00	51.41
MOTA	3222	OH2	TIP3		13.823	-1.538	-3.942	1.00	39.85
ATOM	3225	OH2	TIP3		59.255	3.213	32.873	1.00	76.77
ATOM	3228	OH2	TIP3	183	32.210	13.612	20.027	1.00	60.41
ATOM	3231	OH2	TIP3		72.606	16.267	22.574	1.00	60.78
ATOM	3234	OH2	TIP3		-0.147	5.713	30.877	1.00	50.19
MOTA	3237	OH2	TIP3		-1.207	-4.507	27.969	1.00	65.19
ATOM	3240	OH2	TIP3		81.340	15.584	16.808	1.00	64.48
MOTA	3243	OH2	TIP3		-17.535	3.884	23.785	1.00	57.17
MOTA	3246	OH2	TIP3		27.503	10.697	14.669	1.00	36.11
MOTA	3249	OH2	TIP3		34.585	4.535	27.618	1.00	61.68
ATOM	3252	OH2	TIP3		-3.701	-4.982	9.069	1.00	43.66
ATOM	3255	OH2	TIP3		42.524	7.811	22.390	1.00	34.53
ATOM	3258	OH2	TIP3		52.937	11.764	21.790	1.00	36.19
MOTA	3261	OH2	TIP3		-7.665	8.600	6.358	1.00	59.08
				•		3.000			22.00

•	200
ATOM 3264 OH2 TIP3 195	
3267 OH2 WEDS	86.880 5.187 16.579 1.00 55.88
ATOM 3270 OH2 TTD2	55.377 16.147 20 55.88
ATOM 3273 OH2 TIPS 197	51.394 19 664 22 1.00 48.25
ATOM 3276 OH2 777	20.027 22.988 1.00 46 91
ATOM 2000	28 959 1.00 52 99
ATOM 3303 0112 T1P3 200	26.533 2.319 1.00 40.50
ATOM 2222	2.012 -4.295 1.00 %
More One Tip3 202	3.003 18.397 1 00
NTO: 3208 OH2 TIP3 203	20.752 14.318 1 22
3291 OH2 TIP3 204	-14.418 6 124
ATOM 3294 OH2 TIP3 205	31.488 1.501 - 7.705
A10M 3297 OF 7	10.665 -16.494 15 733
ATOM 3300 OH2 TTD	6.916 -12 200 -1-00 41.42
ATOM 3303 OH2 TTD	-12 650 - 0.160 1.00 62 04
ATOM 3305	11 274
ATOM 3300 002 T1P3 209	11 491 1.588 1.00 49 45
ATOM 3312 ON- TIP3 210	34.037 12.464 -1.531 1.00 44 51
ATOM 2215	13.320 -1.011 1 00
ATOM 3315 OH2 TIP3 212	26.259 7.980 1.00
3318 OH2 TIP3 213	11.633 -1.971 1.00
3321 OH2 TIP3 214	13.599 26 505
ALOM 3324 OHO TEND	5,933 14 957
3327 OH2 TIP3 216	90.599 4.042 6.342
ATOM 3330 OH2 TIDE	50.139 -11.645 10.536
ATOM 3333 Over	66.523 1.024 30.526 1.00 54.64
ATOM 3336 000	74.880
ATOM 3339 CV2	-3.095 20.591 1.00 41 pa
ATOM 2245 11P3 220	5.601 3.142 1.00 52.35
ATOM 224" T1P3 221	35.616 25.022 1.00 29.30
ATOM 33.5	5 381 - 1.00 44 40
ATOM 33.55	10.006 14 081
OH2 TIP3 224	26.814
OH2 TIPE 225	-5.481 20.929 1 20
A10M 3357 OH2 TIP3 226	-1022 -3.876 -0.402 1 00
OH2 TIPE 222	11.220 22 122
ATOM 3363 OH2 TTP3 220	1.011 7.950 59.84
ATOM 3366 OH2 MTD3 6	4.610 -8 037 20 1.00 63.07
ATOM 3369 OH2 TIP2 229 1	1.446 -17.829 12 425 1.00 48.11
ATOM 3372 OUR 72	2 056 - 13.438 1.00 51 35
ATOM 3375 000 11P3 231 57	7 350 1.00 43 90
ATOM 3379 000 11P3 232 43	344 20 - 11.744 1.00 65 45
ATOM 3391 000 TIP3 233 66	723 30.066 1.00 61.52
ATOM 3334 88	15.661 1 00 43
ATOM 2222 1293 235 12	4.257 1.00 61 03
338/ OH2 TTD3 336	- 47.867 1 00
3390 OH2 TIP3 237	-0.425 3.209 1.00
OH2 TIP3 220	28.348 7.731 1.00
	. 792 -8 001 22 - 1.00 53.01
ATOM 3399 OH2 TERS -18.	262 10.614 12.605
ATOM 3402 OH2 TIPS 240 30.	336 11.280 16.000 1.00 51.54
ATOM 240- 11193 241 22	712 -15 810 16.201 1.00 46.53
ATOM 340- 5112 1123 242 29	700 -2.226 1.00 47 20
ATOM 2415 63	297 18.074 1.00 40 10
ATOM 3411 OH2 TIP3 244 61	450 5.497 1.00 49 90
ATOM 3414 OH2 TIP3 245 -0	7.093 11.497 1.00 45.71
341/ OUO mana	2.232 32.172 1 00
on2 11p3 246 66.	6.250 12 150
	0.250 12.159 1.00 34.47



TABLE 3

Atom		Atom	A.A	A.A	x	Y	Z	occ	В	
No.	7	Гуре	Тур	e No.						
MOTA	1	N	GLU	1464	-13.712	16.996	8.424	1.00	61.15	
ATOM	. 3	CA	GLU	1464	-12.478	17.133	7.646	1.00	60.03	
MOTA	4	CB	GLU	1464	-11.465	18.020	8.378	1.00	62.43	
ATOM	5	C	GLU	1464	-11.865	15.766	7.319	1.00	57.36	
MOTA	6	0	GLU	1464	-11.765	15.402	6.145	1.00	60.80	
ATOM	7	N	LEU	1465	-11.466	15.003	8.333	1.00	50.25	
MOTA	9	CA	LEU	1465	-10.899	13.691	8.067	1.00	42.73	
MOTA	10	CB	LEU	1465	-10.097	13.171	9.258	1.00	41.34	
ATOM	11	CG	LEU	1465	-8.571	13.277	9.169	1.00	39.78	
ATOM	12	CD1	LEU	1465	-8.175	14.728	8.977		45.14	
ATOM	13	CD2	LEU	1465	-7.926	12.722	10.426		34.20	·
ATOM	14	С	LEU	1465	-12.009	12.706	7.748	1.00	39.42	
MOTA	15	0	LEU	1465	-13.070	12.719	8.375	1.00	36.63	
MOTA	1.6	N	PRO	1466	-11.821	11.919	6.682		38.54	
ATOM	17	CD	PRO	1466	-10.682	12.019	5.751		37.04	
ATOM	18	CA	PRO	1466	-12.781	10.902	6.232		38.75	
ATOM	1.9	СВ	PRO	1466	-12.176	10.426	4.910		39.49	
ATOM	20	CG	PRO	1466	-10.681	1.0.667	5.109		40.64	
ATOM	21	C	PRO	1466	-12.859	9.756	7.246		39.08	
ATOM	22	0	PRO	1466	-11.834	9.283	7.748		41.23	
ATOM	23	N	GLU	1467	-14.064	9.278	7.513		37.11	
ATOM	25	CA	GľŪ	1467	-14.247	8.213	8.482		35.96	
ATOM	26	CB	GLU	1467	-15.725	8.123	8.863		39.90	
ATOM	27	CG	GLU	1467	-16.334	9.410	9.417		46.64	
ATOM	28	CD	GLU	1467	-17.823	9.280	9.694		51.50	
ATOM	29	OE1	GLU	1467	-18.294	8.135	9.854		54.17	
ATOM	30	OE2	GLU	1467	-18.529	10.315	9.756		53.39	
ATOM	31	C	GLU	1467	-13.794	6.865	7.939		33.77	
ATOM	32	0	GLU	1467	-13.885	6.632	6.740		36.27	
MOTA	33	N	ASP	1468	-13.291	5.991	8.813		29.80	
MOTA	35	CA	ASP	1468	-12.869	4.649	8.409		28.19	
ATOM	36	CB	ASP	1468	-11.362	4.567	8.120		27.83	
MOTA	37	CG	ASP	1468	-10.942	3.223	7.507		27.78	
ATOM	38	OD1	ASP	1468	-11.689	2.225	7.592		25.64	
ATOM	39		ASP	1468	-9.836	3.165	6.935		27.59	
ATOM	40	C	ASP	1468	-13.244	3.672	9.512		28.05	
ATOM	41	0	ASP	1468	-12.462	3.404	10.437	1.00		
ATOM	42	N	PRO	1469	-14.446	3.089	9.403		29.07	
ATOM	43	CD	PRO	1469	-15.401	3.311	8.298		29.93	
ATOM	44	CA	PRO	1469	-14.981	2.124	10.365		28.65	
ATOM	45	CB	PRO	1469	-16.235	1.615	9.659	1.00		
ATOM	46	CG	PRO	1469	-16.690	2.811	8.879	1.00		
ATOM	47	C	PRO	1469	-14.029	0.974	10.687	1.00		
ATOM	48	0	PRO	1469	-14.136	0.364				
ATOM	49	И	ARG	1470	-13.128	0.666	11.748	1.00		
ATOM	51	CA	ARG	1470			9.758	1.00		
	<b>-</b> -	CA	ANG	74.0	-12.161	-0.414	9.947	1.00	∠6.64	



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**ATOM** NE ARG 114 1475 -11.655 12.317 18.954 1.00 45.65 **ATOM** 116 CZARG 1475 -10.447 12.599 18.484 1.00 41.31 ATOM 117 NH1 ARG 1475 -9.420 1.00 35.94 12.686 19.318 ATOM 120 NH2 ARG 1475 -10.253 12.673 17.172 1.00 42.37 **ATOM** 123 C ARG 1475 -12.114 8.232 23.641 1.00 35.29 ATOM 124 ARG -11.094 8.178 0 1475 24.318 1.00 37.28 **ATOM** 125 N **ASP** 1476 -13.304 7.931 24.129 1.00 35.37 **ATOM** 127 CA ASP 1476 -13.468 7.570 25.526 1.00 36.97 **ATOM** 128 CB ASP 1476 -14.952 7.586 25.896 1.00 39.47 ATOM 129 CG ASP 1476 -15.748 6.501 25.205 1.00 40.02 MOTA 130 OD1 ASP 1476 -15.221 5.809 24.320 1.00 41.08 **ATOM** 131 OD2 ASP 1476 -16.926 6.327 25.571 1.00 47.00 ATOM 132 C ASP 1476 -12.850 6.225 25.894 1.00 36.07 MOTA 133 ASP 0 1476 -12 830 5.842 27.066 1.00 36.26 ATOM 134 N ARG 1477 -12.382 5.495 24.888 1.00 36.94 **ATOM** 136 CA ARG 1477 -11.766 4.189 25.104 1.00 35.22 **ATOM** 137 CB ARG 1477 -12.081 3.268 23,925 1.00 34.29 ATOM ARG 138 CG 1477 -13.546 3.056 23.675 1.00 32.23 ATOM 139 CD ARG 1477 -14.206 2.434 24.879 1.00 30.56 **ATOM** 140 NE ARG 1477 -14.426 3.419 25.925 1.00 31.86 **ATOM** 142 CZARG 1477 -14.730 3.126 27.182 1.00 33.09 ATOM 1.43 NH1 ARG 1477 -14.855 27.563 1.858 1.00 35.00 ATOM 146 NH2 ARG 1477 -14.904 4.101 28.053 1.00 29.62 MOTA 149 C ARG 1477 -10.2624.270 25.271 1 00 35.51 ATOM 1.50 0 ARG 1477 -9.621 3.290 25.637 1.00 35.44 ATOM 151 N LEU 1478 -9.704 5.444 25.023 1.00 34.59 **ATOM** i53 CA LEU 1478 1.00 36.35 -8.270 5.630 25, 329 ATOM 154 CB LEU 1478 -7.750 6.254 23.840 1.00 36.41 ATOM 155 CG LEU 1478 -6.250 6.185 23.55€ 1.00 37.19 CD1 LEU MOTA 156 1478 -5.791 4.728 23.479 1.00 34.63 MOTA 157 CD2 LEU 1478 -5.959 6.914 22.251 1 00 34.88 ATOM 158 C LEU 1478 -7.901 6.517 26.325 1.00 38.74 ATOM 159 LEU 0 1478 .8.146 7.733 26.309 1.00 41.20 ATOM VAL 160 N 1479 -7.311 5.907 27.355 1.00 36.92 ATOM CA VAL 162 1479 -6.885 6.622 28.560 1.00 35.79 **ATOM** VAL 163 CB 1479 -6.929 5.693 29.780 1.60 35.81 ATOM 164 CG1 VAL 1479 -6.579 6.453 31.032 1.00 40.11 **ATOM** CG2 VAL 165 1479 -8.302 5.056 29.907 1.00 35.59 MOTA VAL 166 C 1479 28.362 -5.438 7.118 1.00 36.60 ATOM VAL 167 0 1479 -4.479 6.369 28.583 1.00 33.48 ATOM 168 LEU N 1480 -5.282 8.372 27.938 1.00 39.09 ATOM 170 CA LEU 1480 -3.949 8.932 27.675 1.00 42.05 MOTA 171 CB LEU 1480 -4.040 10.277 26.952 1.00 41.08 **ATOM** 172 CG LEU 1480 -4.633 10.286 25.529 1.00 39.28 MOTA 173 CD1 LEU 1480 -4.766 11.720 25.051 1.00 40.04 MOTA 174 CD2 LEU 1480 -3.758 9.489 24.582 1.00 39.66 ATOM 175 С LEU 1480 -3.001 9.027 28.867 1.00 41.51 **ATOM** 176 0 LEU 1480 -3.312 9.637 29.886 1.00 41.73 ATOM 177 N GLY 1481 -1.817 8.444 28.697 1.00 40.68 MOTA 179 CA GLY 1481 -0.849 8.439 29.775 1.00 41.28 **ATOM** 180 С GLY 1481 0.412 9.225 29.529 1.00 43.08 **ATOM** 181 GLY 0 1481 0.474 10.147 28.701 1.00 45.65

Δn	гом					
		182		LYS	1482	1 401
	MOT	184		LYS	1482	8.825 30.219 1 00 42 54
	MO	185		LYS	1482	9.453 30.128 1.00 42 74
	OM	186	CG	LYS	1482	3.070 8 842 31 220
	OM	187	CD	LYS	1482	5.155 8.979 30.954 1.00 53 33
AT		188	CE	LYS	1482	5.867 7.716 31.382 1 00 56 ca
ATO		189	NZ	LYS	1482	5.3/3 6.518 30 607 1 00 5
ATO		193	C	LYS	1482	5.320 30 955 1 00
ATO		194	0	LYS	1482	3.552 9.422 28.806 1.00
ATC	MC	195	N	PRO	1483	3.55/ 8.422 28.111 7.00
ATC		196	CD	PRO		4.259 10.521 28 481 7 3
ATO		197	CA	PRO	1483	4.339 11.798 29 208 1 20 44.06
ATO		198		PRO	1483	5.005 10.573 27 208 1 25
ATO		199		PRO	1483	5.590 12 004 7 1.00 44.07
ATO		200	~		1483	4.630 12 720 1.00 43.17
ATO		201	_		1483	6.172
NOTA	-	202	'		1483	6.853 9.300 27 116 1.00 43.47
ATOM		204	~-		1484	6.408 9.003 25.120 1.00 43.76
ATOM		205			1484	7.512 9.045 1.00 41.71
ATOM	_	06			1484	6.964 6.903 23.863 1.00 38.05
ATOM	_			EU j	L484	5.001 5.003 24.927 1.00 33.38
ATOM	. ~		CD1 L		484	5.258 4.014 25.770 1.00 31.95
ATOM	_		CD2 L		484	6.750 5 706 24.975 1.00 27.41
ATOM	-				484	8 603 3.336 26.953 1.00 29.64
ATOM	_				484	24.855 1.00 40.09
ATOM				LY 1	485	9.945 23.960 1.00 41.74
ATOM				Y 1	485	10 976
ATOM	2:			γ 1.	485	11 261 - 24 512 1.00 50 32
ATOM	21		) GI	Y 14	185	11 026 1- 24.697 1.00 54 65
ATOM	21		GL.	U 14	86	11 745 25.770 1.00 54 73
ATOM	21	_	A GL	U 14	86	13 001 23.647 1.00 59 07
ATOM	21	_		U 14	86	13 400 43.666 1.00 61.01
ATOM	22	-	GL		86	-2.040 24.275 1 00 ca s-
	22		GLI			22.295 1 00 62 46
ATOM	22		. GL			23.5/0 21.949 1 00 64 10
ATOM	224	4 C2	A GL			10.975 12.892 21.519 1 00 62 20
ATOM	225	c c	GLY			10.792 13.522 20.236 1 00 59 07
ATOM	226	0	GLY			11.469 12.881 19 044 1 22
ATOM	227	N	ALA			11.447 13.426 17 950
ATOM	229	CA				12.0/3 11.714 19.239 1 00 57 10
ATOM	230	CB		148		12.721 11.016 18.140 1.00 55 75
ATOM	231	C	ALA	148		9.804 18 663
ATOM	232	0	ALA	148	-	11.690 10.601 17.110
ATOM	233	N	PHE	148		11.92/ 10.626 15 913
ATOM	235	CA	PHE			10.509 10.241 17 599 1 00
ATOM	236	CB	PHE	148		9.401 9.807 16 721 1 00
ATOM	237	CG		1489		8.857
ATOM	238		PHE PHE	1489		9.880 7.373 17.132 1.00 51.18
ATOM	239	CDI	PHE	1489		10.641
ATOM	240	CD2	PHE	1489		10.096 6.612 15.0046.81
ATOM	241	CET	PHE	1489		11.585 6 000 13.964 1.00 48.30
ATOM	242		PHE	1489		11.040 5 600
ATOM	242	CZ	PHE	1489		11.794 5 226 13.363 1.00 48.23
	-43	С	PHE	1489		8.261 10.25
						8.281 10.814 16.748 1.00 54.90
CCCD /n n						

ATOM	244	0	PHE	1489	7.199	10.565	16.184		59.10
MOTA	245	N	GLY	1490	8.431	11.908	17.504		53.55
ATOM	247	CA	GLY	1490	7.432	12.958	17.611	1.00	50.20
ATOM	248	С	GLY	1490	6.745	12.844	18.942	1.00	49.82
ATOM	249	0	GLY	1490	7.266	12.161	19.837	1.00	50.95
MOTA	250	N	GLN	1491	5.614	13.514	19.124	1.00	49.53
MOTA	252	CA	GLN	1491	4.922	13.441	20.395	1.00	49.16
ATOM	253	CB	GLN	1491	3.927	14.590	20.564	1.00	51.74
MOTA	254	CG	GLN	1491	3.439	14.796	21.994	1.00	64.00
MOTA	255	CD	GLN	1491	2.545	16.039	22.180	1.00	71.35
MOTA	256	OE1	GLN	1491	2.534	16.922	21.352	1.00	77.94
ATOM	257	NE2	GLN	1491	1.824	16.083	23.289	1.00	76.51
MOTA	260	С	GLN	1491	4.207	12.083	20.505	1.00	45.94
MOTA	261	0	GLN	1491	. 3.151.	11.869	19.919	1.00	48.02
MOTA	262	N	VAL	1492	4.848	11.129	21.184	1.00	41.00
MOTA	264	CA	VAL	1492	4.293	9.810	21.421	1.00	37.44
ATOM	265	CB	VAL	1492	5.235	8.665	21.025	1.00	34.74
MOTA	266	CG1	VAL	1492	4.593	7.325	21.285	1.00	28.97
ATOM	267	CG2	VAL	1492	5.632	8.769	19.553	1.00	35.78
MOTA	268	C	VAL	1492	4.014	9.621	22.901	1.00	38.67
MOTA	269	0	VAL	1492	4.907	9.769	23.735	1.00	38.62
ATOM	270	И	VAL	1493	2.776	9.276	23.250	1.00	39.98
MOTA	272	CA	VAL	1.493	2.423	9.062	24.653	1.00	37.79
ATOM	273	CB	LAV	1493	1.257	9.970	25.093	1.00	37.36
ATOM	274	CG1	VAL	1493	1.489	11.403	24.689	1.00	39.11
ATOM	275	CG2	VAL	1493	-0.074	9.480	24.555	1.00	38.99
ATOM	276	C	VAL	1493	2.052	7.603	24.877	1.00	36.38
ATOM	277	0	VAL	1493	1.759	6.874	23.945	1.00	37.73
MOTA	278	N	LEU	1494	2.094	7.176	26.123	1.00	35.42
ATOM	280	CA	LEU	1494	1.718	5.817	26.483	1.00	33.65
ATOM	281	CB	LEU	1494	2.536	5.291	2 <b>7</b> .670	1.00	29.88
ATOM	282	CG	LEU	1494	2.117	3.945	28.279	1.00	30.31
MOTA	283	CD1	LEU	1494	2.103	2.844	27.244	1.00	30.83
MOTA	284	CD2	LEU	1494	3.049	3.574	29.400	1.00	32.12
MOTA	285	C	LEU	1494	0.260	5.934	26.870	1.00	34.27
ATOM	286	0	LEU	1494	-0.168	6.994	27.348	1.00	34.85
ATOM	287	N	ALA	1495	-0.527	4.898	26.608	1.00	32.20
MOTA	289	CA	ALA	1495	-1.930	4.954	26.980	1.00	29.71
ATOM	290	CB	ALA	1495	-2.724	5.722	25.930	1.00	25.48
MOTA	291	C	ALA	1495	-2.499	3.567	27.183	1.00	28.85
ATOM	292	0	ALA	1495	-1.826	2.563	26.998	1.00	27.28
ATOM	293	N	GLU	1496	-3.743	3.519	27.615	1.00	32.20
MOTA	295	CA	GLU	1496	-4.413	2.250	27.824	1.00	33.34
ATOM	296	CB	GLU	1496	-4.735	2.063	29.301	1.00	35.65
ATOM	297	CG	GLU	1496	-3.521	1.962	30.198	1.00	39.14
ATOM	298	CD	GLU	1496	-3.899	2.045	31.663	1.00	42.57
MOTA	299		GLU	1496	-4.469	3.083	32.061	1.00	42.59
ATOM	300	OE2	GLU	1496	-3.646	1.069	32.407	1.00	42.76
ATOM	301	С	GLU	1496	-5.692	2.274	26.994	1.00	33.40
MOTA	302	0	GLU	1496	-6.439	3.261	27.017	1.00	34.36
MOTA	303	N	ALA	1497	-5.875	1.247	26.177	1.00	31.67
ATOM	305	CA	ALA	1497	-7.051	1.168	25.351	1.00	31.23

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	TOM 3	06 CE	ALA 14	77 .
	TOM 3	07 C	ALA 149	0.750 23 952 3 24
	TOM 30	0 80	ALA 149	0.168 25 074
	rom 30	9 N		-7.599 -0.954 26 361
AT	TOM 31			-9.218 0.602 36 303
	OM 31			-10.222 -0.294 26 054
	'OM 31			-11.294 0.453 1.00 35.89
AT	OM 31			12.267 -0.553
ATC				-10.663 1 316 25.300 1.00 32.95
ATO			1496	-11.656 2 363 28.770 1.00 35.29
ATO		_	ILE 1498	-10.953 -0.932
ATO			ILE 1498	-11.571 -0.327 -1.00 38.79
ATC			GLY 1499	-10 oro 0.227 24.877 1.00 37 46
ATO			GLY 1499	711 F44 7 25.559 1.00 43 14
ATO		C	GLY 1499	-10 673
ATO		0	GLY 1499	-9 921 23.298 1.00 49 69
ATO		N	LEU 1500	-10 720 -1203 23.387 1.00 51 47
ATO		CA	LEU 1500	24.223 1 00 40 6-
ATOM			LEU 1500	21/03 20.973 1 00 40 65
ATOM		CG	LEU 1500	27.50. 21.185 1.00 49 96
		CD1	LEU 1500	7.504 -1.703 21.167 1 00 40 55
ATOM	. 42,5	CD2 1	LEU 1500	2.217 21.284 1 00 47 47
ATOM		C I	EU 1500	7.638 -0.883 19.899 1 00 47 3
MOTA		0 1	EU 1500	20.535 4.027 20.275 1.00 40 45
ATOM		N P	RO 1505	70.480 -5.145 20.806 1 00 47 00
ATOM		CD p	RO 1505	25.284 1 00 50 75
ATOM	334	CA P	RO 1505	13.8// -7.173 25 220
ATOM	335	CB P	RO 1505	14.19/ -4.825 25 770
ATOM	336		RO 1505	13.348 -5.521 25.627 1 00 46 -
MOTA	337	-	₹0 1505	13.216 -6.944 25 040
ATOM	338	O pr		13.904 -4.396 27 225
ATOM	339	N AS	5	-13.883 -3 202 27 531
ATOM	341	CA AS		43.040 -5.363 20 102
ATOM	342	CB AS		-13.337 -5.053 29 407 1.00 42.10
ATOM	343 (	G AS		-14.202 -5.893 30 434
ATOM		D1 AS		-15.657 -5.493 30 305
ATOM	345 N	D2 AS		-15.999 -4.309 30 407
ATOM	348 C			-16.529 -6.478 30 360 1
ATOM	349 O		0	-11.863 -5.251 29 836 1.00 SI.15
ATOM	350 N			-11.487 -5.343 31 000
ATOM	352 C			-11.029 -5.284 20.005
MOTA	353 C		•	-9.594 -5.466 28 276
ATOM	354 C		•	-9.111 -6.650 28 143
ATOM	355 CI		- • •	-9.327 -7.003
MOTA	356 NE			-8.402 -8.300 - 1.00 64.52
ATOM			1507	-8.592 -9.404 23.363 1.00 71.17
ATOM			1507	-8.030 -9.000 1.00 76.52
ATOM		1 ARG	1507	-7.219 -0.006 31.689 1.00 81.64
ATOM		2 ARG	1507	-8.340 -11 000 32.375 1.00 83.30
ATOM	365 C	ARG	1507	-8.871 -4.334 1.00 84.44
ATOM	366 0	ARG	1507	-9.227 -2.605 1.00 43.46
ATOM	367 N	VAL	1508	-7.912 -2.742 27.440 1.00 42.73
ATOM	369 CA	VAL	1508	-7 143 29.265 1.00 40 RA
	370 CB	VAL	1508	-6 70c 28.830 1.00 38 27
				-6.786 -1.604 29.961 1.00 34.90

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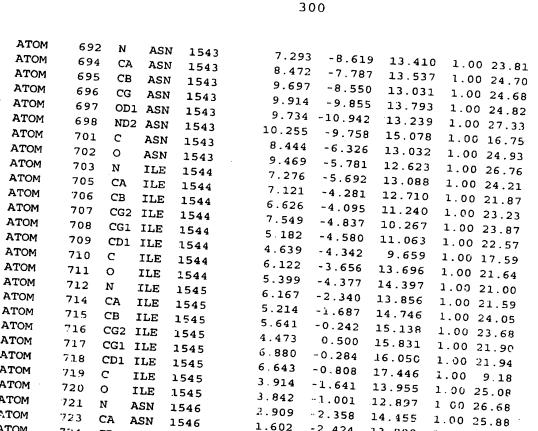
ATOM	371	CG1.	VAL	1508	-8.038	-1.124	30.646	1.00	41.81
MOTA	372	CG2	VAL	1508	-5.850	-2.226	30.944	1.00	35.89
ATOM	373	C	VAL	1508	-5.874	-3.147	28.211	1.00	36.81
ATOM	374	0	VAL	1508	-5.371	-4.191	28.637	1.00	35.13
ATOM	375	N	THR	1509	-5.393	-2.465	27.180	1.00	36.04
ATOM	377	CA	THR	1509	-4.184	-2.854	26.485	1.00	33.31
ATOM	378	CB	THR	1509	-4.503	-3.254	25.025	1.00	33.79
ATOM	379	OG1	THR	1509	-5.511	-4.275	25.014	1.00	33.98
ATOM	381	CG2	THR	1509	-3.259	-3.774	24.321	1.00	32.78
MOTA	382	С	THR	1509	-3.268	-1.627	26.453	1.00	32.37
MOTA	383	0	THR	1509	-3.718	-0.533	26.113	1.00	31.97
ATOM	384	N	LYS	1510	-2.015	-1.786	26.884	1.00	32.96
ATOM	386	CA	LYS	1510	-1.071	-0.673	26.828	1.00	33.25
MOTA	387	CB	LYS	1510	0.157	-0.902	27.699	1.00	34.65
ATOM	388	CG	LYS	1510	-0.093	-0.909	29.197	1.00	39.64
ATOM	389	CD	LYS	1510	1.237	-1.105	29.913	1.00	43.51
ATOM	390	CE	LYS	1510	1.110	-1.949	31.173	1.00	48.42
ATOM	391	NZ	LYS	1510	0.399	-1.256	32.287	1.00	53.03
ATOM	395	С	LYS	1510	-0.646	-0.550	25.370	1.00	32.26
.ATOM	396	0	LYS	1510	-0.240	-1.533	24.736	1.00	30.20
ATOM	397	N	VAL	1511	-0.760	0.665	24.849	1.00	32.28
ATOM	399	CA	VAL	1511	0.436	0.980	23.472	1.00	30.73
MOTA	400	CB	VAL	1511	-1.738	1.140	22.666	1.00	32.25
ATOM	401	CG1	VAL	1511	-2.566	0.147	22.723	1.00	29.00
MOTA	402		VAL	1511	-2.549	2.347	23.193	1.00	29.17
MOTA	403	С	VAL	1511	0.329	2.307	23.423	1.00	30.91
ATOM	404	0	VAL	1511	0.445	3.008	24.433	1.00	31.94
MOTA	405	N	ALA	1512	0.842	2.658	22.250		27.30
ATOM	407	CA	ALA	1512	1.550	3.914	22.094	1.00	
MOTA	408	CB	ALA	1512	2.921	3.694	21.493	1.00	
ATOM	409	С	ALA	1512	0.698	4.769	21.181	1.00	
ATOM	410	0	ALA	1512	0.116	4.271	20.228	1.00	
ATOM	411	N	VAL	1513	0.605	6.054	21.484	1.00	
ATOM	413	CA	VAL	1513	-0.192	6.984	20.688	1.00	
MOTA	414	CB	VAL	1513	-1.359	7.613	21.522	1.00	
ATOM	415	CG1	VAL	1513	-2.218	8.522	20.650	1.00	
ATOM	416		VAL	1513	-2.214	6.542	22.159	1.00	
ATOM	417	С	VAL	1513	0.674	8.108	20.107		31.21
ATOM ATOM	418	0	VAL	1513	1.370	8.816	20.834 18.784	1.00	
ATOM ATOM	419	N	LYS	1514	0.631	8.225		1.00	
ATOM, ATOM	421	CA	LYS	1514	1.342	9.258	18.037	1.00	
	422	CB	LYS	1514	1.831	8.692	16.707	1.00	
ATOM	423	CG	LYS	1514	2.835	7.586	16.872	1.00	
ATOM	424	CD	LYS	1514	3.025	6.807	15.599	1.00	
ATOM	425	CE	LYS	1514	3.457	7.710	14.438	1.00	
ATOM	426	NZ	LYS	1514	4.598	8.622	14.755	1.00	
ATOM	430	C	LYS	1514	0.304	10.345	17.761	1.00	
ATOM	431	0	LYS	1514	-0.806	10.037	17.299	1.00	
ATOM	432	N Ca	MET	1515	0.673	11.596	18.028	1.00	
ATOM	434	CA	MET	1515	-0.207	12.747	17.835	1.00	
ATOM	435	CB	MET	1515	-0.901	13.098	19.145	1.00	
ATOM	436	CG	MET	1515	0.075	13.428	20.255	1.00	39.II

ATOM 437 CD	
ATOM 151	-0.766
ATOM 438 CE MET 1515	13.612 21.799 7.00
ATOM 439 C MET 1515	11.937 22.087 1 00
ATOM 440 0 MET 1515	13.939 17.391 1 00
ATOM LEU 1516	13.905 17.445
ATOM CA LEU 1516	14.962 16.872 1 00
ATOM CB LEU 1516	16.175 16.448 1 20
ATOM THE CG LEW 1516	16.917 15.374 1 00
ATTOM CD1 LEU 1516	16.254 14.036 7.00
ATOM CD2 LEU 1516	17.104 13.285
ATOM 115 LEU 1516	16.102 13.265 1 02
ATOM 1516	17.119 17.631 1 00
ATOM 450 N LYS 1517	16.927 18.703 1 22
ATOM ATO	18.174 17.402 1 33.99
ATOM AS: CB LYS 1517	19.193 18 416
ATOM ASS CG LYS 1517	19.668 18.344 1 20
ATOM LYS 1517	18.559 18.529 1 00 05.34
ATOM CE LYS 1517	3.046 18.935 17.929 1 40 -
ATOM LYS 1517	17.851 18.197 7 30
ATOM 462 C LYS 1517	- I I I I I I I I I I I I I I I I I I I
ATOM 463 W LYS 1517	0 303 20 18.139 1.00 65 97
ATOM 465 G	0 776 21 - 17.053 1.00 64 50
ATOM 466 CD 1518	-0 107 2- 19.098 1.00 69 20
ATOM 467 0 SER 1518	-0.002: 22 - 18.9/4 1.00 71.00
ATOM 468 0 358 1518	0 144 25.322 20.202 1.00 59 90
ATOM 460 1 1518	70 799 77 17.718 1.60 74 60
ATOM 471 CA ASP 1519	1 417 23.604 17.006 1.00 77 44
ATOM 472 CP 300	1 799 24 - 1.422 1.00 75 04
ATOM 473 C 1519	3 726 27 10.264 1.00 75 40
ATOM 474 0 707	1 912 00 10 10 10 17 10
ATOM 475 N N N N N N N N N N N N N N N N N N N	2.374 24 075 14.958 1.00 75.88
ATOM 477 CA 313	1.486 22 265 - 1.00 77.52
ATOM 478 CB 313	1 574 25 14.956 1.00 74 30
ATOM 479 C 313	0.930 20.079 14 258 1.00 72.83
ATOM 480 0 373	0.889 22 153 14.010 1.00 73.06
ATOM 481 N TUD 152	-0.096 22 850
483 CA THR 1521	1.440 22 015 - 1.00 /3.48
A10M 484 CD my-	0.858 22 652 - 4.00 69.15
485 OGI TUD	1.950 23 110 - 1.00 /0.05
ATOM 487 CG2 mrm	2.505 21 960 - 1.00 70.21
ATOM 488 C THR 1521	3.053 23.815 10 1.00 72.71
A10M 489 0 mm	-0.015 21 616
A10M 490 N CT	0.015 20 443
492 Ch Cr	-0.782 22.026 0 THE T.00 72.38
493 CB GUI 1500	-1.623 21.081 7.815 1.00 69.70
ATOM 494 C GLU 1522	-2.478 21.800 6.761 1.00 67.41
A10M 495 O GLU 1500	7.168 1.00 70.01
ATOM 496 N LYS 1523	7.006 1 00 64.50
ATOM 498 CA LYS 1523	0.512 20.419 6.827 1 20 63.76
ATOM 499 CB LYS 1523	1.483 19.502 6.240 1.00 60.75
500 CG LYS 1523	2.782 20.230 5.883 1.00 58.57
	3.909 19.318 5.361 1.00 62.47
SSSD/55145, v01	00 62.47

MOTA	501	CD	LYS	1523	3.459	18.461	4.168	1.00	63.35
ATOM	502	CE	LYS	1523	4.633	17.700	3.559	1.00	66.57
MOTA	503	NZ	LYS	1523	4.210	16.733	2.498	1.00	69.56
MOTA	507	С	LYS	1523	1.763	18.441	7.281	1.00	55.98
MOTA	508	0	LYS	1523	1.790	17.251	6.972	1.00	56.37
MOTA	509	N	ASP	1524	1.960	18.885	8.517	1.00	52.16
ATOM	511	CA	ASP	1524	2.211	17.980	9.630	1.00	48.91
MOTA	512	CB	ASP	1524	2.487	18.762	10.915	1.00	50.87
MOTA	513	CG	ASP	1524	3.865	19.401	10.928	1.00	53.00
MOTA	514	OD1	ASP	1524	4.004	20.511	11.489	1.00	53. <b>7</b> 7
MOTA	515	OD2	ASP	1524	4.816	18.785	10.394	1.00	56.30
MOTA	516	С	ASP	1524	1.032	17.031	9.831	1.00	45.34
MOTA	517	0	ASP	1524	1.221	15.858	10.176	1.00	45.63
MOTA	518	N	LEU	1525	-0.176	17.530	9.593	1.00	40.15
MOTA	520	CA	LEU	1525	-1.368	16.715	9.711	1.00	39.38
MOTA	521	CB	LEU	1525	-2.624	17.588	9.633	1.00	41.66
MOTA	522	C.G	LEU	1525	-4.020	16.937	9.585	1.00	42.75
ATOM	523	CD1	LEU	1525	-4.245	15.945	10.727	1.00	42.97
ATOM	524	CD2	LEU	1525	-5.058	18 026	9.644	1.00	42.24
MOTA	525	C	LEU	1525	-1.340	15.699	8.575	1.00	39.77
MOTA	526	O	LEU	1525	-1.509	14.506	8.813	1.00	39.11
ATOM	527	N	SER	1526	-1.062	16.172	7.361	1.60	39.64
MOTA	529	CA	SER	1526	-0.998	15.320	6.181	1.00	40.65
ATOM	530	CB	SER	1526	-0.541	16.105	4.947		43.32
ATOM	531	OG	SER	1526	-1.398	17.190	4.656		52.41
ATOM	533	C,	SER	1526	-0.015	14.201	6.383	1.00	39.12
MOTA	534	O	SER	1526	-0.346	13.038	6.198	1.00	41.75
MOTA	535	N	ASP	1527	1.203	14.553	ö.769	1.00	38.30
MOTA	537	CA	ASP	1527	2 244	13.552	6.969	1.00	39.28
MOTA	538	CB	ASP	1527	3.531	14.208	7.471	1.00	41.16
ATOM	539	C'G	ASP	1527	4.218	15.069	6.404	1.00	45.20
ATOM	540	OD1	ASP	1527	3.861	14.972	5.198	1.00	43.25
ATOM	541	OD2	ASP	1527	5.132	15.840	6.788	1.00	45.93
ATOM	542	C	ASP	1527	1.788	12.443	7.903	1.00	37.34
ATOM	543	0	ASP	1527	1.867	11.259	7.557	1.00	37.24
ATOM	544	N	LEU	1528	1.224	12.935	9.036	1.00	35.88
MOTA	546	CA	LEU	1528	0.728	11.874	10.009	1.00	35.07
MOTA	547	CB	LEU	1528	0.185	12.606	11.242	1.00	34.38
MOTA	548	CG	LEU	1528	-0.146	11.789	12.491	1.00	35.86
MOTA	549	CD1	LEU	1528	1.009	10.845	12.820	1.00	34.83
MOTA	550	CD2	LEU	1528	-0.435	12.711	13.642	1.00	29.98
ATOM	551	C	LEU	1528	-0.351	10.977	9.374	1.00	33.31
MOTA	552	0	LEU	1528	-0.342	9.756	9.552	1.00	34.55
ATOM	553	N	ILE	1529	-1.236	11.575	8.585	1.00	32.16
ATOM	555	CA	ILE	1529	-2.306	10.829	7.924	1.00	30.94
MOTA	556	CB	ILE	1529	-3.304	11.757	7.178	1.00	
MOTA	557	CG2	ILE	1529	-4.388	10.926	6.521	1.00	
A'TOM	558	CG1	ILE	1529	-3.953	12.723	8.169	1.00	
ATOM	559	CD1	ILE	1529	-4.877	13.736	7.526	1.00	
ATOM	560	С	ILE	1529	-1.684	9.856	6.947	1.00	
ATOM	561	0	ILE	1529	-2.058	8.683	6.912	1.00	
MOTA	562	N	SER	1530	-0.703	10.331	6.191	1.00	

ATOM		64	CA S	SER	1530		0.00	0.7	0 40					
ATOM	_	65	CB S	SER			1.10		9.49				32.	
MOTA	5	66	OG S	SER	1530		0.59		10.30	_			35.	
ATOM	5	68	C S	ER	1530		0.62		11.50		_		41.	
ATOM	56	59	0 5	ER	1530		0.47		8.26	•			29.	
ATOM	5	70	N G	LU	1531				7.14				26.	
ATOM	57	72		LU	1531		1.28		8.46			.00	23.	86
ATOM	57	73 (		LU	1531		1.91		7.36			.00	23.	86
ATOM	57	4 (		LU	1531		2.72		7.89			.00	25.6	69
ATOM	57			LU	1531		3.50		6.80		)1 1		23.6	
ATOM	57		El G		1531		4.34		7.319		8 1	.00	26.0	03
ATOM	57		)E2 G		1531		4.92		6.473		2 1		25.9	
MOTA	57			ւՄ	1531		4.43		8.549				26.5	
ATOM	57	9 C		บัน	1531		0.90		6.325				25.4	
ATOM	58			ET	1532		1.200		5.126	8.22			23.6	
ATOM	58:		A ME		1532		-0.289		6.788				26.3	
ATOM	58:	_	B ME		1532		-1.365		5.898	9.04			26.5	
ATOM	584						-2.473		6.720				24.8	
ATOM	589	_			1532 1532		-3.645		5.889	10.19	1 1.	oo ·	27.4	7
ATOM	586						-4.969		5.899	10.86	01.		28.4	
ATOM	587		ME		1532		-5.178		8.102	9.576			24.4	5
ATOM	588	_	ME		1532		-1.923		5.076	7.863			28.3	
ATOM	589		GL		1532		-2.048		3.850	7.933			27.9	
ATOM	591				1533		-2.221		5.760	6.762			28.9	
ATOM	592				1533		-2.732	•	5.111	5.565			30.32	
ATOM	593				1533		-2.983		6.143	4.476			25.40	
ATOM	594				1533	·	-4.064		7.127	4.852			6.09	
ATOM	595	OE			1533		-5.402		6.461	5.119			5.89	
ATOM	596		2 GLT		1533		-5.913		5.745	4.240			7.24	
ATOM	597	C	GLU		1533		-5.964		6.662	6.209		0 3	0.00	)
ATOM	598	o	GLU		1533		-1.723		4.089	5.093			1.64	
ATOM	599	N	MET		1533		-2.080		2.983	4.706			3.57	
ATOM	601	CA	MET		1534		-0.455		4.472	5.166			3.57	
ATOM	602	CB	MET		1534		0.664		3.618	4.793			2.86	
ATOM	603	CG	MET		L534		1.957		4.390	5.003			2.89	
ATOM	604	SD	MET	_	L534		3.159		3.559	4.851			9.27	
ATOM	605	CE	MET		1534		3.577		3.513	3.164			1.24	
ATOM	606	C	MET		.534		5.153	4	4.319	3.204			1.97	
ATOM	607	0	MET		.534		0.670	:	2.373	5.681			L.84	
ATOM	608	N	MET	-	534		0.816		1.250	5.198			3.78	
ATOM	610	CA	MET		535		0.509	2	2.571	6.982	1.0	3 3 0	).36	
ATOM	611	CB			535		0.469	נ	l.453	7.902	1.00			
ATOM	612	CG	MET		535		0.419	1	. 946	9.352	1.00	24	75	
ATOM	613	SD	MET		535		1.717	2	2.540	9.850	1.00	) 21	50	
ATOM	614	CE	MET		535		1.722	2	.764	11.628	1.00	22	97	
ATOM	615	C	MET		535		1.681	4		11.727	1.00	23	90	
ATOM	616		MET		535		-0.725	0	.540	7.572	1.00	30	32	
ATOM	617	0	MET		535		-0.636	- 0	.694	7.706	1.00			
ATOM	619	N Ca	LYS		536		-1.823		.135	7.104	1.00			
ATOM		CA	LYS		536		-3.011		.364	6.732	1.00			
ATOM	620	CB	LYS		36		-4.176		. 289	6.413	1.00	25		
ATOM	621	CG	LYS		36		-4.689		.080	7.579	1.00			
	622	CD	LYS	15	36		-5.810		.979	7.127	1.00			
										÷ ·	00	±9.	. 0 )	

ATOM	623	CE	LYS	1536	-6.414	3.717	8.288	1.00 23.50
MOTA	624	NZ	LYS	1536	-7.469	4.668	7.850	1.00 23.53
ATOM	628	C	LYS	1536	-2.765	-0.542	5.530	1.00 29.09
ATOM	629	0	LYS	1536	-3.127	-1.708	5.550	1.00 34.02
ATOM	630	N	MET	1537	-2.141	-0.009	4.488	1.00 29.03
ATOM	632	CA	MET	1537	-1.869	-0.792	3.288	1.00 30.13
ATOM	633	CB	MET	1537	-1.315	0.111	2.177	1.00 31.96
ATOM	634	CG	MET	1537	-2.304	1.114	1.589	1.00 35.15
MOTA	635	SD	MET	1537	-3.757	0.380	0.787	1.00 41.18
ATOM	636	CE	MET	1537	-3.026	-0.360	-0.666	1.00 43.05
ATOM	637	С	MET	1537	-0.905	-1.946	3.531	1.00 30.22
ATOM	638	0	MET	1537	-1.118	-3.051	3.045	1.00 30.88
ATOM	639	N	ILE	1538	0.164	-1.686	4.275	1.00 30.91
MOTA	641	CA	ILE	1538	1.192	-2.701	4.536	1.00 30.29
ATOM	642	CB	ILE	1538	2.429	-2.082.	5.221	1.00 28.64
ATOM	643	CG2	ILE	1538	3.493	-3.142	5.453	1.00 29.84
MOTA	644	CG1	ILE	1538	3.025	-1.030	4.287	1.00 32.82
MOTA	645	CD1	ILE	1538	4.358	-0.446	4.763	1.00 38.38
ATOM	646	C	ILE	1538	0.759	-4.000	5.237	1.00 29.07
ATOM	647	0	ILE	1538	1.229	-5.078	4.876	1.00 28.30
ATOM	648	N	GLY	1539	-0.178	-3.925	6.174	1.00 27.61
ATOM	650	CA	GLY	1539	-0.592	-5.147	6.849	1.00 26.22
ATOM	651	С	GLY	1539	0.273	-5.484	8.055	1.00 25.67
ATOM	652	0	GLY	1.539	1.345	-4.906	8.241	1.00 28.05
MOTA	653	N	LYS	1540	-0.150	-6.483	8.819	1.00 23.80
ATOM	655	CA.	LYS	1540	0.532	-6.876	10.046	1.00 21.77
ATOM	656	CB	LYS	1540	-0.491	-7.436	11.045	1.00 20.04
ATOM	657	CG	LYS	1540	-1.505	-6.435	11.480	1.00 24.45
ATOM	658	CD	LYS	1540	-2.472	-6.997	12.488	1.00 32.57
ATOM	659	CE	LYS	1540	-3.516	-5.946	12.882	1.00 35.05
MOTA	660	NZ	LYS	1540	-2.959	-4.850	13.733	1.00 39.81
ATOM	664	С	LYS	1540	1.669	-7.862	9.958	1.00 20.19
ATOM	665	0	LYS	1540	1.671	-8.738	9.099	1.00 21.80
MOTA	666	N	HIS	1541	2.626	-7.722	10.876	1.00 19.98
ATOM .	668	CA	HIS	1541	3.770	-8.626	11.000	1.00 22.43
ATOM	669	CB	HIS	1541	4.854	-8.374	9.965	1.00 22.34
ATOM	670	CG	HIS	1541	5.892	-9.455	9.923	1.00 20.68
MOTA	671	CD2	HIS	1541	5.906	-10.654	9.295	1.00 20.60
MOTA	672	ND1	HIS	1541	7.074	-9.382	10.633	1.00 23.67
MOTA	674	CE1	HIS	1541	7.771	-10.490	10.444	1.00 23.35
ATOM	675	NE2	HIS	1541	7.087	-11.278	9.634	1.00 22.04
ATOM	677	C	HIS	1541	4.385	-8.477	12.376	1.00 27.21
MOTA	678	0	HIS	1541	4.538	-7.367	12.885	1.00 31.33
ATOM	679	N	LYS	1542	4.726	-9.619	12.958	1.00 29.25
ATOM	681	CA	LYS	1542	5.319	-9.698	14.285	1.00 30.39
MOTA	682	CB	LYS	1542	5.660	-11.151	14.610	1.00 33.76
MOTA	683	CG	LYS	1542		-11.370	15.994	1.00 42.16
ATOM	684	CD	LYS	1542		-12.833	16.230	1.00 49.69
MOTA	685	CE	LYS	1542		-13.499	14.988	1.00 57.71
ATOM	686	NZ	LYS	1542		-14.904	15.237	1.00 62.05
ATOM	690	С	LYS	1542	6.515	-8.808	14.462	1.00 27.21
ATOM	691	0	LYS	1542	6.690	-8.232	15.522	1.00 29.68
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ATOM **ATOM** ATOM ATOM ATOM ATOM ATOM 1.602 **ATOM** -2.424 724 13.800 CB 1.00 24.61 ASN 1546 0.944 ATOM -3.793 725 14.005 CG 1.00 23.18 ASN 1546 1.759 ATOM -4.923 .13.434 726 OD1 ASN 1.00 21.54 1546 1.884 ATOM -5.059 727 12.214 ND2 ASN 1.00 21.52 1546 2.319 -5.748 **ATOM** 14.313 730 С 1.00 18.83 ASN 1546 0.646 ATOM -1.368 14.292 731 1.00 23.02 0 ASN 1546 0.739 ATOM -0.911 15.429 732 1.00 25.66 N LEU 1547 -0.285 -1.014 ATOM 13.422 734 CA 1.00 24.45 LEU 1547 -1.336 ATOM -0.041 13.692 735 CB LEU 1.00 24.27 1547 -1.819 ATOM 0.553 12.360 736 1.00 18.04 CG LEU 1547 -3.012 ATOM 1.515 12.343 737 CD1 LEU 1.00 19.96 1547 -2.630 ATOM 2.928 12.842 738 CD2 LEU 1.00 10.60 1547 -3.555 **ATOM** 1.570 10.924 739 C 1.00 16.44 LEU 1547 -2.469 -0.826 **ATOM** 14.384 740 1.00 26.95 0 LEU 1547 -2.835 **ATOM** -1.934 13.956 741 1.00 27.38 N LEU 1548 -2.998 ATOM -0.260 743 15.460 1.00 26.61 CA LEU 1548 -4.063 -0.902 **ATOM** 744 16.222 CB 1.00 26.25 LEU 1548 -3.717 -0.951 ATOM 745 17.721 1.00 22.48 CG LEU 1548 -2.370 -1.553 ATOM 18.117 746 1.00 20.24 CD1 LEU 1548 -2.282 ATOM -1.656 19.616 747 CD2 LEU 1.00 19.27 1548 -2.175 -2.929 ATOM 748 17.492 1.00 19.23 C LEU 1548 -5.401 ATOM -0.198 749 16.017 0 1.00 26.75 LEU 1548 -6.447 -0.837 ATOM 750 16.036 1.00 25.56 N GLY 1549 ~5.367

-6.607

-6.319

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MOTA	755	N	ALA	1550	-7.369	4.143	15.530	1.00 27.34
MOTA	757	CA	ALA	1550	-7.212	5.582	15.414	1.00 25.85
MOTA	758	CB	ALA	1550	-6.925	5.947	13.978	1.00 23.09
MOTA	759	С	ALA	1550	-8.430	6.353	15.897	1.00 26.58
MOTA	760	0	ALA	1550	-9.562	5.866	15.797	1.00 28.26
ATOM	761	N	CYS	1551	-8.182	7.551	16.429	1.00 26.30
ATOM	763	CA	CYS	1551	-9.227	8.471	16.899	1.00 28.29
ATOM	764	CB	CYS	1551	-8.966	8.952	18.342	1.00 27.12
ATOM	765	SG	CYS	1551	-9.101	7.681	19.630	1.00 27.09
MOTA	766	С	CYS	1551	-9.092	9.646	15.934	1.00 28.57
MOTA	767	0	CYS	1551	-8.156	10.436	16.044	1.00 26.80
MOTA	768	N	THR	1552	-9. <b>96</b> 6	9.699	14.933	1.00 29.27
MOTA	770	CA	THR	1552	-9.889	10.736	13.921	1.00 29.30
MOTA	771	CB	THR	1552	- 9 . 779	10.110	12.495	1.00 27,19
ATOM	<b>7</b> 72	OG1	THR	1552	-10.978	9.393	12.191	1.00 26.68
ATOM	774	CG2	THR	1552	-8.629	9.133	12.414	1.00 27.00
ATOM	775	C	THR	1552	-11.045	11.716	13.905	1.00 29.86
ATOM	<b>7</b> 76	0	THR	1552	-10.918	12.838	13.403	1.00 30.69
ATOM	777	N	GLN	1553	-12.201	11.268	14.369	1.00 31 21
ATOM	779	CA	GLN	1553	-13.374	12.124	14.329	1.00 34.31
ATOM	780	CB	GLN	1553	-14.641	11.279	14.147	1.00 33.00
ATOM	781	CG	GLN	1553	-14.714	10.530	12.820	1.00 34.68
MOTA	782	CD	GLN	1553	-14.584	11.453	3.1.617	1.00 39.26
ATOM	783	OE1	GLN	1553	-15.300	12.449	11.506	1.00 43.55
MOTA	784	NE2	GLN	1553	-13.668	11.129	1.0.718	1.00 37.56
ATOM	787	C	GLN	1553	-13.502	13.040	15.526	1.00 36.86
MOTA	788	0	GLN	1553	-13.030	12.714	16.613	1.00 34.88
ATOM	789	N	ASP	1554	-14.122	14.195	15.290	1.00 40.73
MOTA	791	CA	ASP	1554	-14.369	15.202	16.3:3	1.00 42.49
MOTA	792	CB	ASP	1554	-15.693	14.913	17.028	1.00 46.26
MOTA	793	CG	ASP	1554	-16.907	15.174	16.153	1.00 51.14
MOTA	794	OD1	ASP	1554	-17.686	16.097	16.488	1.00 57.62
ATOM	795	OD2	ASP	1554	-17.092	14.463	15.146	1.00 55.72
ATOM	796	C	ASP	1554	-13.249	15.299	17.336	1.00 42.31
MOTA	797	0	ASP	1554	-13.443	14.955	18.501	1.00 43.61
MOTA	798	N	GLY	1555	-12.077	15.753	16.902	1.00 41.03
MOTA	800	CA	GLY	1555	-10.960	15.864	17.823	1.00 37.98
MOTA	801	C	GLY	1555	-9.605	15.674	17.167	1.00 38.30
ATOM	802	0	GLY	1555	-9.533	15.478	15.953	1.00 37.28
ATOM	803	N	PRO	1556	-8.511	15.693	17.961	1.00 37.62
ATOM	804	CD	PRO	1556	-8.575	15.755	19.429	1.00 37.23
MOTA	805	CA	PRO	1556	-7.123	15.533	17.500	1.00 33.79
ATOM	806	CB	PRO	1556	-6.296	15.748	18.773	1.00 33.33
MOTA	807	CG	PRO	1556	-7.254	16.353	19.770	1.00 36.99
ATOM	808	С	PRO	1556	-6.891	14.134	16.990	1.00 33.57
MOTA	809	0	PRO	1556	-7.378	13.175	17.568	1.00 32.10
ATOM	810	N	LEU	1557	-6.168	14.031	15.884	1.00 33.23
MOTA	812	CA	LEU	1557	-5.859	12.745	15.300	1.00 34.20
ATOM	813	CB	LEU	1557	-5.173	12.950	13.944	1.00 32.88
ATOM	814	CG	LEU	1557	-4.674	11.716	13.183	1.00 29.78
ATOM	815		LEU	1557	-5.810	10.730	12.943	1.00 29.22
ATOM	816	CD2	LEU	1557	-4.085	12.161	11.880	1.00 28.17

AT	OM 0			
ATO	J.,	C LEU	1557	
ATO	0.10	O LEU	1557	2 047 16.225 1.00 36.29
	34	N TYR	1558	-5 427 16.580 1.00 37.50
ATC	021	CA TYR	1558	-4 610 10.765 16.658 1.00 35.35
ATC		CB TYR	1558	-5 323 3.890 17.495 1.00 33.09
ATO	02.5	CG TYR	1558	5.516 18.805 1.00 34.16
ATO	~ L 3	CD1 TYR	1558	6 364 10.629 19.806 1.00 34.40
ATO		CE1 TYR	1558	20.088 20.771 1.00 33 33
ATO	•	CD2 TYR	1558	21.663 1.00 34 52
ATO	- L,	CE2 TYR	1558	-4.426 11.655 19.757 1 00 37 30
ATO		CZ TYR	1558	-4.488 12.715 20.640 1 00 30 44
ATON			1558	25.494 12.762 21.587 1 00 35 12
ATOM		_	1558	-5.561 13.848 22 431 1 20 2
ATOM		<b>~</b>	1558	-4.379 8.627 16.700 1 00 3
ATOM			1559	-5.329 7.980 16 255 1 20 m
ATOM				-3.109 8.321 16 468 1 00 a-
ATOM			1559	-2.727 7.115 15 753 1 00 29.60
ATOM	_		1559	-1.647 7.435
ATOM	_	ICO	.559	-1.281 6 1.0
ATOM	839 C	· · · · · ·	559	-2.147 0 525
ATOM	840 0		559	-2.238 6.300
ATOM		77	559	-1.169 6.252
ATOM			560	-3.067 5 005 1-389 1.00 24.97
ATOM			560	-2.777 4.000 1.00 25.91
ATOM			560	-4.081 3.535
ATOM			560	-3.785 2.744
ATOM	• • -		560 .	-5.028 4.707
ATOM	847 CI	Ol ILE 19	60	-6 450 4 30 12.84
ATOM	848 C	ILE 15	60	1.955 2.225
ATOM	849 O	ILE 15	60	-2 445 2 to 17.467 1.00 30.61
ATOM	850 N		61	-0.698 2.211 16.636 1.00 31.41
ATOM	852 CA		61	0.222 1.770 1.00 30.26
ATOM	853 CB	VAL 15	61	1 466 2 435
ATOM	854 CG:	1 VAL 15	61	1.030 3.700 1.00 30.18
ATOM		2 VAL 15	61	3.188 15.475 1.00 20.60
	856 C	VAL 156	51	0.663
ATOM	857 O	VAL 156	51	0.333 0.870 18.588 1.00 27.40
ATOM	858 N	GLU 156		1 301 1.128 19.742 1.00 29.33
ATOM	860 CA	GLU 156		1 952 18.279 1.00 24.75
ATOM	861 CB	GLU 156		2 426 19.308 1.00 22.64
ATOM	862 CG	GLU 156		18.676 1.00 17 97
ATOM	863 CD	GLU 156	2	1 000 24 33
ATOM	864 OE1	GLU 156		17.383 1.00 26 00
ATOM	865 OE2	GLU 156		17.507 1.00 33 33
ATOM	866 C	GLU 156		16.722 1.00 25 62
ATOM	867 O	GLU 156		2.885 -0.534 20.259 1 00 25 25
ATOM	868 N	TYR 1563		3.638 0.355 19.899 1.00 23 83
ATOM	870 CA			2.897 -1.023 21.491 1.00 22
ATOM				3.805 -0.539 22 512 1 00 22
ATOM	0.00			3.045 -0.428 23 829 1 00 25
ATOM	0.7.			3.868 0.008 25 009 1 00
ATOM	874 CE1			4.581 1.196 24 976 1.00 27.72
ATOM				5.303 1.620 26.069 1.00 33.61
	875 CD2	TYR 1563		3.908 0.702
				26.176 1.00 25.77
CCCC				

PCT/US97/14885

MOTA	876	CE2	TYR	1563	4.626	-0.344	27.267	1.00	26.81
ATOM	877	CZ	TYR	1563	5.329	0.845	27.210	1.00	32.81
ATOM	878	OH	TYR	1563	6.091	1.271	28.276	1.00	40.16
MOTA	880	С	TYR	1563	4.989	-1.487	22.675	1.00	28.73
MOTA	881	0	TYR	1563	4.815	-2.704	22.735	1.00	27.05
MOTA	882	N	ALA	1564	6.189	-0.908	22.743	1.00	29.89
ATOM	884	CA	ALA	1564	7.453	-1.634	22.916	1.00	28.50
ATOM	885	CB	ALA	1564	8.392	-1.349	21.721	1.00	27.54
ATOM	886	C	ALA	1564	8.036	-1.092	24.229	1.00	27.05
ATOM	887	0	ALA	1564	8.790	-0.129	24.249	1.00	31.20
ATOM	888	N	SER	1565	7.650	-1.706	25.333	1.00	27.11
MOTA	890	CA	SER	1565	8.062	-1.251	26.652	1.00	28.91
ATOM	891	CB	SER	1565	7.501	-2.152	27.729	1.00	27.33
MOTA	892	OG	SER	1565	8.108	-3.419	27.650	1.00	26.58
ATOM	894	C	SER	1565	9.530	-1.085	26.915	1.00	30.19
ATOM	895	0	SER	1565	9.897	-0.330	27.810	1.00	33.44
MOTA	896	N	LYS	1566	10.368	-1.801	26.178	1.00	30.99
ATOM	898	CA	LYS	1566	11.798	-1.708	26.410	1.00	30.50
ATOM	899	CB	LYS	1566	12.452	-3.082	26.335	1.00	30.38
ATOM	900	CG	LYS	1566	12.037	-3.943	27.507	1.00	27.83
ATOM	901	CD	LYS	1566	12.605	-5.339	27.457	1.00	32.36
ATOM	902	CE	LYS	1566	12.345	-6.024	28.784	1.00	30.57
ATOM	903	NZ	LYS	1566	12.651	-7.460	28.722	1.00	34.82
ATOM	907	С	LYS	1566	12.526	-0.678	25.573	1.00	30.39
ATOM	908	0	LYS	1566	13.755	-0.567	25.640	1.00	32.53
ATOM	909	N	GLY	1567	11.753	0.1.27	24.851	1.00	29.45
MOTA	911	CA	GLY	1567	12.319	1.184	24.035	1.00	29.17
ATOM	912	C	$GL \cdot Y$	1567	13.079	0.742	22.806	1.00	28.14
MOTA	913	Ů	GLY	1567	12.875	-0.364	22.324	1.00	27.70
MOTA	914	N	ASN	1568	13.975	1.601	22.320	1.00	29.48
ATOM	916	CA	ASN	1568	14.754	1.308	21.121	1.00	30.00
ATOM	917	CB	ASN	1568	15.271	2.591	20.464	1.00	28.53
ATOM	918	CG	ASN	1568	16.342	3.285	21.281	1.00	30.13
ATOM	919	OD1	ASN	1568	17.305	2.670	21.730	1.00	31.50
MOTA	920	ND2	ASN	1568	16.212	4.591	21.420	1.00	30.91
MOTA	923	C	ASN	1568	15.892	0.333	21.352	1.00	28.83
MOTA	924	0	ASN	1568	16.371	0.201	22.472	1.00	29.87
MOTA	925	N	LEU	1569	16.346	-0.300	20.274	1.00	27.43
MOTA	927	CA	LEU	1569	17.417	-1.291	20.323	1.00	29.95
MOTA	928	CB	LEU	1569	17.511	-2.022	18.972	1.00	28.96
MOTA	929	CG	LEU	1569	18.508	-3.173	18.797	1.00	30.82
MOTA	930	CD1	LEU	1569	18.431	-4.211	19.939	1.00	28.31
MOTA	931	CD2	LEU	1569	18.244	-3.819	17.461	1.00	25.70
ATOM	932	С	LEU	1569	18.805	-0.779	20.754	1.00	29.74
ATOM	933	0	LEU	1569	19.530	-1.484	21.447	1.00	28.35
ATOM	934	N	ARG	1570	19.179	0.427	20.341	1.00	31.42
MOTA	936	CA	ARG	1570	20.485	0.985	20.703	1.00	32.81
MOTA	937	CB	ARG	1570	20.639	2.395	20.115	1.00	
MOTA	938	CG	ARG	1570	21.922	3.091	20.543	1.00	
MOTA	939	CD	ARG	1570	21.918	4.581	20.212	1.00	
MOTA	940	NE	ARG	1570	20.700	5.272	20.649	1.00	
ATOM	942	CZ	ARG	1570	20.393	5.595	21.912	1.00	

Amos.	
ATOM 943 NH1 ARG 157	0
A10M 946 NU2 ND	5.304 32 02-
949 C NOC 15	19.245 6 227 25 1.00 51.30
ATOM 950 0 NDG	20.620 1.034 32 323
ATOM 951 N CTT	21.548 0.455 25.250 1.00 35.61
ATOM 953 CA CIT	19.677 1.724 22 252
ATOM 954 CB CUI	19.637
ATOM 955 CG CLU 15/1	18.403 2 662 24.311 1.00 37.35
ATOM 956 CD CIV	18.407 4 118 24.725 1.00 41.36
ATOM 957 OR-	17.048 4 933 24.267 1.00 49.97
ATOM 950 070	15 997 24.459 1.00 59 14
ATOM OF - 13/1	17 042 24.595 1.00 59 21
ATOM 900 - GLU 1571	19 502 24.446 1.00 59 41
ATOM 961 W GLU 1571	20 327 24.948 1.00 37 00
ATOM OCA TYR 1572	18 750 25.892 1.00 37 70
ATOM 25 CA TYR 1572	44.400 1 00
ATOM OCT THE 1572	17 571 -1.766 24.878 1.00 32 73
ATOM 255 CG TYR 1572	23,995 1 00 3
ATOM 1572	15.376 -3.973 24.309 1 00 27
ATOM 1572	10.392 -4.378 25.187 1 00 an
ATOM 968 CD2 TYR 1572	25.458 1 00 00
ATOM CE2 TYR 1572	-4.941 23.703 1 66 25
970 CZ TYR 1572	23.969 1.00 05
ATOM 9/1 OH TYR 1572	16.659 24.852 1 00 05
773 C TYR 1572	20.732 -7.985 25.143 1 00 25
974 O TVP 1572	-2.504 -2.505 -24 00.
975 N LEU 1572	20.400 -3.309 25 205
ATOM 977 CA TEST	20.692 -2.338 23 912
ATOM 978 CB 1771	21.970 -3.033
ATOM 979 CG 1771	22.487 -3.018 32 075
ATOM 980 CD1 I FIX	21.833 -3.880 1.00 29.86
71 OM 981 CD2 1 mrs	. 22.339 -3.448 30.040 1.00 23.37
982 C TETT 4	42.129 -5 354 1.00 16.57
ATOM 983 O TEST	22.997 -2.417 24 655
ATOM 984 N CTN	23.752 -3.134 35 335
ATOM 986 CA CLN 15/4	23.003 -1.090 24 72-
ATOM 987 CB CLN 1374	23.942 -0.399 35 500 1.00 37.26
ATOM 988 CG GVV	23.844 7 110 25.608 1.00 37.50
ATOM OPP CT	24.526 1 502 25.394 1.00 36.96
ATOM 990 OF GIVE	24.289 3.054 24.113 1.00 39.10
ATOM 991 ME2 CV	23.697 3.796 23.801 1.00 40.63
ATOM 994 C 574	24.736 3 400 24.595 1.00 38.68
ATOM 995 0	23.687 -0.750 -22.625 1.00 38.62
ATOM 996 N 1574	24 500 27.073 1.00 38 27
ATOM COO TO ALA 1575	22 422 27.801 1.00 39 42
ATOM 900 TA ALA 1575	22 021 - 27.469 1.00 38 pg
ATOM 1000 - ALA 1575	20 551 28.831 1.00 39 51
ATOM 1001 ALA 1575	22 304 2 49.024 1.00 36 89
ATOM 1000 ALA 1575	22 006 - 29.275 1.00 40 80
ATOM 1004 ARG 1576	22 957 30.417 1.00 44 52
ATOM 1004 CA ARG 1576	23 149 -3.317 28.395 1.00 39 11
ATOM 1005 CB ARG 1576	28.768 1 00 35.11
Amor: 1006 CG ARG 1576	22.234 -5.669 28.019 1 00 30
ATOM 1007 CD ARG 1576	-5.518 28.472 1 00 no
-	19.838 -6.352 27.687 1.00 39.73
SSSD/55145 v01	00 3/.8/

**ATOM** 1008 NE ARG 1576 18.489 -6.260 28.235 1.00 41.03 ATOM 1010 CZARG 1576 17.830 -5.123 28.436 1.00 43.27 ATOM -3.961 1011 NH1 ARG 1576 18.399 28.143 1.00 42.64 **ATOM** 1014 NH2 ARG 1576 16.573 -5.152 28.877 1.00 46.13 ATOM 1017 C ARG 1576 24.604 -5.076 28.612 1.00 39.77 **ATOM** 1018 0 ARG 1576 24.978 -6.256 28.623 1.00 40.25 **ATOM** 1019 Ν ARG 1577 25.428 -4.042 28.501 1.00 40.39 MOTA 1021 CA ARG 1577 26.866 -4.194 28.388 1.00 40.42 **ATOM** 1022 CB ARG 1577 -2.871 27.485 27.952 1.00 37.67 MOTA 1023 CG ARG 1577 27.247 -2.477 26.526 1.00 36.22 ATOM 1024 CD ARG 1577 27.857 -1.113 26.287 1.00 35.55 MOTA 1025 NE ARG 1577 27.971 -0.797 24.866 1.00 38.72 MOTA 1027 CZARG 1577 28.395 0.369 24.384 1.00 37.57 1028 MOTA NH1 ARG 1577 28.754 1.352 25.205 1.00 37.49 MOTA 1031 NH2 ARG 1577 28.449 0.562 23.074 1.00 39.58 **ATOM** 1034 C ARG 1577 27.449 -4.548 29.760 1.00 42.45 **ATOM** 1035 0 ARG 1577 26.878 -4.180 30.801 1.00 42.57 **ATOM** 1036 N PRO 1578 28.564 -5.296 29.797 1.00 43.36 ATOM 1037 CD PRO 1578 29.270 -5.985 28.692 1.00 42.43 **ATOM** 1038 CA PRO 1578 29.159 -5.648 31.082 1.00 43.08 ATOM 1039 CB PRO 1578 30.225 -6.676 30.709 1.00 40.33 **ATOM** 1040 CG PRO 1578 30.600 -6.300 29.331 1.00 40.71 ATOM 1041 С -4.373 PRO 1578 29.768 31.666 1.00 42.44 **ATOM** 1042 PRO 0 1578 30.261 -3.525 30.922 1.00 41.24 MOTA 1043 N PRO 1579 29.705 -4.205 32.993 1.00 44.57 **ATOM** 1044 PRO CD 1579 29.169 -5.143 33.994 1.00 46.68 **ATOM** 1045 CA PRO 1579 30.251 -3.017 33.654 1.00 44.89 ATOM 1046 CB PRO 1579 30.088 -3.356 35.134 1.00 45.31 MOTA 1047 CG PRO 1579 28.865 -4.224 35.142 1.00 44.45 MOTA 1048 C PRO 1579 31.711 -2.767 33.289 1.09 45.17 **ATOM** 1049 0 PRO 1579 32.620 -3.257 33.953 1.00 47.72 **ATOM** 1050 N ALA 1592 19.075 -5.384 32.475 1.00 49.23 **ATOM** 1052 CA ALA 1592 20.500 -5.078 32.354 1.00 50.33 **ATOM** 1053 CB ALA 1592 20.954 -4.184 33.503 1.00 51.83 **ATOM** 1054 C ALA 1592 21.412 -6.308 32.251 1.00 50.65 **ATOM** 1055 0 ALA 1592 22.621 -6.166 32.044 1.00 51.55 MOTA 1056 N ALA 1593 20.849 -7.505 32.409 1.00 49.06 **ATOM** 1058 CA ALA 1593 21.638 -8.735 32.294 1.00 48.07 **ATOM** 1059 CB ALA 1593 1.00 47.87 20.773 -9.953 32.579 **ATOM** 1060 C ALA 1593 22.258 -8.840 30.891 1.00 47.59 **ATOM** 1061 ALA 0 1593 21.664 -8.426 29.894 1.00 49.09 **ATOM** 1062 N GLN 1594 23.465 -9.388 30.830 1.00 47.30 ATOM 1064 GLN CA 1594 24.186 -9.553 29.569 1.00 45.32 ATOM 1065 CB GLN 1594 25.576 -10.118 29.837 1.00 44.82 MOTA 1066 CG GLN 1594 26.523 -9.166 30.542 1.00 49.34 MOTA 1067 CD GLN 1594 27.751 -9.877 31.111 1.00 52.40 **ATOM** 1068 OE1 GLN 1594 28.264 -10.847 30.537 1.00 51.16 ATOM 1069 NE2 GLN 1594 28.209 -9.408 32.265 1.00 54.00 **ATOM** 1072 C GLN 1594 23.474 -10.432 28.539 1.00 45.00 **ATOM** 1073 0 GLN 1594 22.780 -11.393 28.876 1.00 45.28 MOTA 1074 N LEU 1595 23.684 -10.104 27.273 1.00 45.08 **ATOM** 1076 CA LEU 1595 23.084 -10.828 26.169 1.00 44.65

*	TOR					
	<b>m</b>	1077		LEU	1595	22.758 -9.864 25.00-
		1078		LEU	1595	25.023 1 00 43 00
		1079	CD1	LEU	1595	25.295 1.00 43 22
	TOM	1080	CD2		1595	21.855 -7.563 24.564 1 00 41 35
	TOM :	1081	С		1595	20.276 -9.510 24 919 1 25
A.	rom ;	1082	0			24.044 -11.885 25 605 3
A7	rom 1	1083	N	~	1595	25.252 -11.661 25 633
AT		085	CA		1596	23.511 -12.050 1.00 44.62
AT		086	CB		1596	24.325 -14 153 -1 1.00 45.71
AT		087		_	1596	23.633 -15 405 1.00 45.30
	-	089	OG		1596	22.401 -15 607 1.00 46.19
AT	^			SER 1	.596	24.557 -13 000 2-1.00 44.03
AT	_	090		SER 1	596	23 801 23.366 1.00 45 09
AT	^	091	N ,	SER 1	597	25 475 22.707 1.00 45 03
		93	CA .	SER 1	597	- +3·/38 // 855
ATO		94	CB S		597	
ATO		95	OG g		597	20.921 -15.643 21 065 1 22
ATC		97			597	27.976 -15.516 22 002 3
ATC	)M 10	98	_		597	24.526 -15.076 20 633 1 55
ATO		99				24.233 -14.498 19.573
ATO	M 11				98	23.767 -16.025 21 170 1.00 45.51
ATO		_			98	22.551 -16 454
ATO		~ ~			98	21.978 - 7.7.7.5
ATO					98	21.374 - 10 (42
ATOM	M 110	`		YS 15		20.450 -19 605
ATON			E Ly			20.05420
ATOM			IZ LY		98	21.219 -21.55
ATOM				'S 159	98	21 521 4- 19.334 1.00 30 59
ATOM	_	_		S 159	98 .	20 940 4-
			As			21 442 19.548 1 00 36 39
ATOM			A AS	P 159	9	***************************************
ATOM			B AS			
ATOM		6 C	G AS			20.635 -12.898 23 220
ATOM	111	7 01	Ol AS			20.143 -13.838 24 320 7 3-
ATOM	1118	3 01	D2 ASI	2 159		~~ <del>***********************************</del>
ATOM	1119	) C	ASI			19.256 -14.691 24.073
ATOM	1120	0	ASE			20./// -12.430 20 802 3
ATOM	1121		LEU			19.846 -11.945 20 153 7.00
ATOM	1123					22.046 -12.070
ATOM	1124					22.439 -11 050
ATOM	1125					23.921 -10 605
ATOM	1126			1600	)	24.341 -10.000
ATOM		CD		1600		25.857 -9 023 1.00 29.24
ATOM	1127		2 LEU	1600		23.666 -9.73
ATOM	1128	C	LEU	1600		22 126
ATOM	1129	0	LEU	1600		· · · · · · · · · · · · · · · · · · ·
	1130	N	VAL	1601		22 430 30 17.418 1.00 31.23
ATOM	1132	CA	VAL	1601		44.743 )/ 863 3 66 -
ATOM	1133	CB	VAL	1601		+2.431 16 510 7 00 -
ATOM	1134	CG1	VAL	1601		22.827 -14.600 16 261
ATOM	1135		VAL	1601		22.46/ -15.108 14 995
ATOM	1136	C	VAL			24.326 -14.474 16 363 1 36
ATOM	1137	ō	VAL	1601		20.642 -13.340 16 310 1 3
ATOM	1138	N	SER	1601		20.152 -13.151 15 191 1 19
ATOM	1140	CA		1602		19.904 -13.635 17 382 1 00 28.55
		CA	SER	1602		18 450 -13 736
						17.318 1.00 27.07
CCCD/cca						



MOTA	1141	CB	SER	1602	17.899 -14.362	18.584	1.00 29.97
ATOM	1142	QG	SER	1602	16.488 -14.202	18.673	1.00 38.86
MOTA	1144	С	SER	1602	17.864 -12.327	17.093	1.00 27.45
ATOM	1145	0	SER	1602	16.826 -12.181	16.438	1.00 29.38
ATOM	1146	N	CYS	1603	18.504 11.306	17.663	1.00 25.31
ATOM	1148	CA	CYS	1603	18.087 -9.909	17.461	1.00 24.49
MOTA	1149	CB	CYS	1603	19.074 -8.965	18.143	1.00 21.15
MOTA	1150	SG	CYS	1603	18.716 -7.213	18.030	0.50 11.83 PRT1
MOTA	1151	С	CYS	1603	18.155 -9.628	15.961	1.00 26.92
MOTA	1152	0	CYS	1603	17.175 -9.238	15.329	1.00 30.04
ATOM	1153	N	ALA	1604	19.340 -9.833	15.398	1.00 28.35
ATOM	1155	CA	ALA	1604	19.573 -9.611	13.979	1.00 28.00
ATOM	1156	CB	ALA	1604	20.970 10.098	13.588	1.00 25.49
MOTA	1157	C	ALA	1604	18.517 -10.295	13.132	1.00 26.69
ATOM	1158	0	ALA	1604	17.892 -9.646	12.310	1.00 31.40
MOTA	1159	N	TYR	1605	18.270 -11.577	13.399	1.00 26.33
ATOM	1161	CA	TYR	1605	17.286 -12.384	12.666	1.00 24.79
ATOM	1162	CB	TYR	1605	17.209 -13.771	13.300	1.00 23.42
MOTA	1163	CG	TYR	1605	16.132 -14.663	12.742	1.00 29.93
ATOM	1164	CD1	TYR	1605	16.281 -15.298	11.510	1.00 30.00
ATOM	1165	CE1		1605	15.270 -16.097	10.989	1.00 32.29
ATOM	1166	CD2	TYR	1605	14.949 14.859	13.441	1.00 32.69
ATOM	1167	CE2	TYR	1605	13.935 -15.650	12.934	1.00 33.02
ATOM	1168	CZ	TYR	1605	14.091 -16.266	11.713	1.00 34.40
A'TOM	1169	OH	TYR	1605	13.037 -17.023	11.225	1.00 34.18
MOTA	1171	С	TYR	1605	15.885 -11.750	12.572	1.00 26.08
ATOM	1172	C	TYR	1605	15.327 -11.587	11.475	1.00 25.43
ATOM	1173	N	GLN	1606	15.337 -11.366	13.717	1.00 25.38
ATOM	1175	CA	GLN	1606	14.018 -10.737	13.776	1.00 25.47
ATOM	1176	CB	GLN	1606	13.662 -10.424	15.227	1.00 24.21
ATOM	1177	CG	GLN	1606	13.642 -11.636	16.127	1.00 24.37
ATOM	1178	CD	GLN	1606	13.237 -11.279	17.540	1.00 27.16
MOTA	1179	OE1	GLN	1606	12.227 -10.603	17.758	1.00 29.64
ATOM	1180	NE2	GLN	1606	14.033 -11.705	18.507	1.00 30.69
ATOM	1183	C	GLN	1606	13.953 -9.449	12.949	1.00 26.89
ATOM	1184	0	GLN	1606	12.936 -9.136	12.319	1.00 26.40
ATOM	1185	N	VAL	1607	15.030 -8.674	13.000	1.00 27.79
ATOM ATOM	1187	CA	VAL VAL	1607	15.120 -7.430	12.255	1.00 26.35
ATOM	1188	CB		1607	16.408 -6.667	12.625	1.00 24.87
ATOM	1189		VAL	1607	16.556 -5.433	11.752	1.00 25.90
ATOM	1190 1191		VAL	1607	16.382 -6.282	14.094	1.00 17.95
ATOM		C	VAL	1607	15.121 -7.743	10.757	1.00 27.69
ATOM	1192	0	VAL	1607	14.406 -7.093	9.979	1.00 30.85
ATOM	1193	N	ALA	1608	15.902 -8.749	10.355	1.00 24.59
ATOM	1195 1196	CA CB	ALA	1608	15.965 -9.135	8.950	1.00 23.22
			ALA	1608	16.971 -10.227	8.750	1.00 17.65
ATOM ATOM	1197	C	ALA	1608	14.579 -9.589	8.492	1.00 24.58
ATOM	1198 1199	O N	ALA ARG	1608	14.201 -9.372	7.337	1.00 26.22
ATOM	1201	N CA	ARG	1609 1609	13.819 -10.191	9.409	1.00 25.65
ATOM	1201	CB	ARG		12.453 -10.648	9.124	1.00 24.86
ATOM	1202			1609	11.998 -11.660	10.160	1.00 28.15
711 OF	1203	CG	ARG	1609	12.451 -13.050	9.863	1.00 30.10

ATOM 1204 CD 200	•
CD ARG 160	9 77 692
1205 NE ARG 160	-2.003 -13.980 10 722 1 00 -
1207 CZ ARG 160	
ATOM 1208 NH1 ARC 160	10.058 -15.792 10 437 1 22
ATOM 1211 NO	9.800 -15.790 11 740 1 35.69
ATOM 1214 C ARC 151	9.468 -16.678 9.645 1.00 32.47
ATOM 1215 0	11.421 -0.516
ATOM 1216 " ARG 160	9 10.522
ATOM 1212	11.501 .0.502
ATOM 1210 CA GLY 1610	0.522 9.888 1.00 20.88
3max = 1215 C GLY 1610	10 932 7.398 9.789 1.00 21.47
GLY 1610	8.432 1 00 22 55
ATOM 1221 N MET 1617	9.8/2 -6.452 7.688 1.00 22.53
ATOM 1223 CA MET 1500	12.097 -6.558 8 000 - 23.33
1224 CR MPT 35-	12.488 -5.955 6 ROS 1
ATOM 1225	13.991 -5.686 6 801 1 -5
ATOM 1226 an	14.391 -4.470
ATOM 1227 CD	13.362 -3.000 7.052 1.00 27.09
ATOM 1222 - MET 1611	13.665 715 7.330 1.00 22.57
ATOM 1333	12 000 5.612 1.00 21.91
	5.590 1 00 26 57
1230 N GLU 1612	4.553 1 00 24 00
1232 CA GLU 1612	5,710 1 00 37 66
11233 CB CITY 2575	4.632 1 00 25 -
1234 CG GLU 1612	12.120 -10.446 5.024 1.00 26 7
ATOM 1235 CD GLU 1612	11.602 -11.443 4.026 1.00 20
ATOM 1236 DEL CITA	11.796 -12.872 4 477 1 00 29.25
ATOM 1222 1012	11.65R 12 142
ATOM 1220	12.085 -12 922 - 2.00 33.39
ATOM 1239 3	10.354
ATOM 1240 W 1612	9.974 - 9.665 4.305 1.00 27.55
ATOM 1242 TO 171R 1613	9.518 -9.750 1.00 30.04
ATOM 1345 LIK 1613	B. 092 - 9. 545 5.337 1.00 25.13
ATOM 15 11R 1613	7 343 5.133 1.00 21.91
11R 1613	6.462 1 00 21 22
1245 CD1 TYR 1613	4 000 6.335 1.00 17 47
1246 CE1 TYR 1613	5.968 1 00 10 24
ATOM 1247 CD2 TYR 1613	3.610 -9.049 5.872 1.00 10.00
ATOM 1248 CE2 TVP 1613	5.3/3 -7.041 6.600 1 00 14.40
ATOM 1240	4.017 -6.761 6.502 1.00 14.48
ATOM 1000 1013	3.137 -7.775
ATOM 1252 - TOLI	1.779 -7.543
ATOM 1252 - TAN 1813	7 870 7 22 21 91
ATOM 1254 N	7.125 7.024 1.00 22.06
ATOM 1356	8.541
ATOM 1614	R 400
ATOM 1614	9 219 2 4.536 1.00 20.56
7701 1258 CG LEU 1614	9.540 5.392 1.00 18.43
1259 CD1 LEU 1614	3.413 6.707 1 00 15 06
ATOM 1260 CD2 LEU 1614	9.509 -2.571 7.518 1.00 15 70
ATOM 1261 C LEU 1614	7-255 -2.647 6 436 1 33
ATOM 1262 0 LEU 1614	8.793 -4.671 3.066 3.00
ATOM 1263 N ATA 1614	8.156 -3.939 2 294 7 22
ATOM 1265 CD ALA 1615	9.840 -5.397 3.604
ATOM 1266 CD 1015	10 333 5 400 2.004 1.00 24.55
ATOM 1262 -	11.685 -6 000
A10H 1267 C ALA 1615	9 334 6 105 1.254 1.00 18.35
	9.334 -6.107 0.404 1.00 21.97
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ATOM	1268	0	ALA	1615	9.089	-5.642	-0.705	1.00 23.80
ATOM	1269	N	SER	1616	8.704	-7.173	0.893	1.00 22.49
MOTA	1271	CA	SER	1616	7.722	-7.919	0.097	1.00 21.81
ATOM	1272	CB	SER	1616	7.305	-9.179	0.831	1.00 19.78
ATOM	1273	OG	SER	1616	6.382	-8.862	1.851	1.00 23.88
MOTA	1275	С	SER	1616	6.475	-7.071	-0.149	1.00 23.60
ATOM	1276	0	SER	1616	5.733	-7.277	-1.117	1.00 21.74
MOTA	1277	N	LYS	1617	6.217	-6.169	0.789	1.00 25.84
ATOM	1279	CA	LYS	1617	5.078	-5.280	0.705	1.00 23.96
MOTA	1280	CB	LYS	1617	4.555	-4.951	2.099	1.00 20.74
ATOM	1281	CG	LYS	1617	3.843	-6.124	2.750	1.00 23.40
MOTA	1282	CD	LYS	1617	2.509	-6.395	2.081	1.00 28.70
MOTA	1283	CE	LYS	1617	1.714	-7.442	2.809	1.00 31.16
MOTA	1284	NZ	LYS	1617	2.339	-8.767	2.616	1.00 41.91
MOTA	1288	С	LYS	1617	5.409	-4.019	-0.061	1.00 24.25
MOTA	1289	Ö	LYS	1617	4.640	-3.053	-0.022	1.00 25.22
MOTA	1290	N	LYS	1618	6.557	-4.028	-0.748	1.00 24.20
MOTA	1292	CA	LYS	1618	7.014	-2.904	-1.582	1.00 25.15
ATOM	1293	CB	LYS	1618	5.906	-2.507	-2.571	1.00 27.00
ATOM	1294	CG	LYS	1618	5.735	-3.411	-3.790	1.00 29.09
MOTA.	1295	CD	LYS	1618	5.506	-4.864	3.432	1.00 31.82
MOTA	1296	CE	LYS	1618	5.533	-5.752	-4.663	1.00 30.21
MOTA	1297	NZ	LYS	1618	4.231	-5.707	-5.369	1.00 26.34
MOTA	1301	C	LYS	1618	7.466	-1.658	-0.816	1.00 23.50
MOTA	i302	0	LYS	1618	7.537	-0.576	-1.385	1.00 22.10
MOTA	1.303	N	CYS	1619	7.827	-1.821	0.449	1.00 23.72
ATOM	1305	CA	CYS	1619	8.213	-0.693	1.276	1.00 20.89
ATOM	1306	CB	CYS	1619	7.535	-0.814	2.647	1.00 18.41
ATOM	1307	SG	CYS	1619	8.019	0.405	3.894	1.00 26.34
ATOM	1308	С	CYS	1619	9.717	-0.529	1.451	1.00 22.94
MOTA	1309	O	CYS	1619	10.419	-1.487	1.790	1.00 23.20
MOTA	1310	N	ILE	1620	10.197	0.690	1.211	1.00 21.17
MOTA	1312	CA	ILE	1620	11.610	1.039	1.388	1.00 22.35
ATOM	1313	CB	ILE	1620	12.151	1.823	0.172	1.00 17.30
ATOM	1314	CG2	ILE	1620	13.607	2.215	0.393	1.00 8.27
MOTA	1315	CG1	ILE	1620	11.966	0.997	-1.111	1.00 18.27
MOTA	1316	CD1	ILE	1620	12.127	1.803	-2.401	1.00 17.57
ATOM	1317	С	ILE	1620	11.631	1.926	2.652	1.00 25.20
ATOM	1318	0	ILE	1620	10.912	2.932	2.715	1.00 29.69
ATOM	1319	N	HIS	1621	12.398	1.526	3.665	1.00 22.66
ATOM	1321	CA	HIS	1621	12.463	2.254	4.931	1.00 22.78
ATOM	1322	CB	HIS	1621	13.214	1.425	5.980	1.00 22.65
ATOM	1323	CG	HIS	1621	13.024	1.897	7.398	1.00 22.07
ATOM	1324		HIS	1621	12.485	1.280	8.475	1.00 20.50
ATOM	1325	ND1		1621	13.449	3.134	7.842	1.00 23.11
ATOM	1327		HIS	1621	13.182	3.253	9.131	1.00 23.92
MOTA	1328		HIS	1621	12.596	2.144	9.543	1.00 24.44
MOTA	1330	C	HIS	1621	13.110	3.616	4.831	1.00 24.07
MOTA	1331	0	HIS	1621	12.561	4.597	5.306	1.00 24.37
ATOM	1332	N	ARG	1622	14.327	3.639	4.291	1.00 26.42
ATOM	1334	CA	ARG	1622	15.129	4.853	4.130	1.00 24.59
ATOM	1335	CB	ARG	1622	14.289	6.018	3.581	1.00 17.58

Δη	ГОМ										
		1336	CG	ARG	1622	13.8	810 =	765			
		1337	CD	ARG	1622	12.9		.767 2	.163	1.00	13.88
		1338	NE	ARG	1622	12.5			.634	0.50	4.97
		1340	CZ	ARG	1622				. 243	0.50	6.49
	OM 1	1341	NH1	ARG	1622	11.5		852 -0	.145	0.50	3.84
AT		344	NH2		1622	10.7	-	308 0	. 753	0.50	2.25
AT		347	С	ARG	1622	11.3	-	6111.	433	0.50	
ATO		348	0	ARG		15.9			388		2.48 24.72
ATO		349		ASP	1622	16.76			337		
ATC		351		ASP	1623	15.68	35 4.		505		26.90
ATC		352	_		1623	16.43			703	1.00	25.61
ATO		353		ASP	1623	15.92			349	1.00	28.41
ATO		354		ASP	1623	16.89	1 6.			1.00	30.38
ATO		355	OD1		1623	16.42			373	1.00	33.47
ATO		356		ASP	1623	18.12				1.00 4	13.35
ATO				SP	1623	16.49			167	1.00 3	81.88
ATO				SP	1623	16.14				1.00 2	8.86
MOTA				EU	1624	16.95	_		887	1.00 2	8.31
ATOM			CA L	EU	1624	17.087			46	1.00 2	7.81
			CB L		1624	17.149	_		07	1.00 2	7.28
ATOM			CG F		1624	17.118			42 1	.00 2	7.53
ATOM			CD1 L	EU .	1624				16 1	.00 2	7.69
ATOM		64 (	D2 L		1624	15.850		18 9.7	56 1	.00 2	3.77
ATOM		55 (			1624	17.228			05 1	.00 2	9 15
ATOM		66 C			1624	18.340		8 10.00		.00 26	5 27
ATOM		57 N			1625	19.464		3 9.51		.00 25	
ATOM	136	9 c	A AL		.625	18.116	1.59	8 .1.31		.00 23	2.00
ATOM	137		B AL	_	.625	19.164	1.75	0 12.31		.00 19	
MOTA	137			-		19.520	3.23	3 12.47		.00 18	.68
ATOM	137				625	18.575	1.21	4 13.61		00 20	.85
ATOM	137	_		_	625	17.352	1.07			00 20	. 79
ATOM	137			_	626	19.429	0.94	–		00 20	. 75
ATOM	137				626	18.969	0.408			00 22	. 03
ATOM	137				526	20.139	-0.048			00 23	.43
ATOM	1378		AL		526	18.111	1.397			00 22	. 46
ATOM	1379	_	AL		526	17.333	1.006			00 25	. 86
ATOM	1381		ARC		527	18.303	2.685			00 29.	51
ATOM	1382				27	17.503	3.722			00 26.	92
ATOM					27	18.017	5.107			00 27.	30
ATOM	1383				27	18.086	5.287			00 28.	29
ATOM	1384		ARG	16	27	18.255	6.756			0 36.	
ATOM	1385		ARG	16	27	18.548		14.688		0 41.	
ATOM	1387		ARG	16	27	19.779	6.928	13.261		0 39.	94
	1388	NH	L ARG	16:	27	20.826	6.904	12.749	1.0	0 42.	33
ATOM	1391	NH	ARG	162	27	19.976	6.721	13.539	1.0	0 44.	75
ATOM	1394	C	ARG	162		16.029	7.059	11.450	1.0	0 41.5	50
ATOM	1395	0	ARG	162			3.567	16.591	1.0	0 27.4	12
ATOM	1396	N	ASN	162		15.092	3.897	17.333	1.0	0 26.5	3
ATOM	1398	CA	ASN	162		15.850	3.039	15.375	1.0	26.8	2
MOTA	1399	CB	ASN	162		14.534	2.849	14.758	1.00	24.0	Ω.
ATOM	1400	CG	ASN	162		14.569	3.308	13.301	1.00	26.3	0
ATOM	1401		ASN			14.709	4.823	13.167	1.00	25.1	0
ATOM	1402		ASN	162		14.018	5.567	13.844	1 00	28.5	<i>3</i>
ATOM	1405	C	ASN	162		15.599	5.277	12.297	1 00	40.5	y ^
		-	HON	162	ಶ	13.945	1.440	14.862	1 00	22.3	<b>2</b>
									00	24.3	5

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ATOM	1406	0	ASN	1628	13.026	1.084	14.105	1.00 24.66
ATOM	1407	N	VAL	1629	14.473	0.637	15.785	1.00 22.35
ATOM	1409	CA	VAL	1629	13.988	-0.718	16.055	1.00 20.65
ATOM	1410	CB	VAL	1629	15.077	-1.813	15.822	1.00 18.07
ATOM	1411	CG1	VAL	1629	14.612	-3.142	16.398	1.00 11.84
ATOM	1412	CG2	VAL	1629	15.378	-1.977	14.346	1.00 12.65
MOTA	1413	С	VAL	1629	13.625	-0.670	17.536	1.00 24.27
MOTA	1414	0	VAL	1629	14.427	-0.237	18.361	1.00 25.94
ATOM	1415	N	LEU	1630	12.393	-1.031	17.866	1.00 24.99
MOTA	1417	CA	LEU	1630	11.936	-1.010	19.247	1.00 25.50
MOTA	1418	CB	LEU	1630	10.609	-0.252	19.339	1.00 22.79
MOTA	1419	CG	LEU	1630	10.634	1.179	18.789	1.00 17.86
MOTA	1420	CD1	LEU	1630	9.240	1 680	18.654	1.00 18.49
.ATOM	1421	CD2	LEU	1630	11.409	2.100	19.668	1.00 17.63
MOTA	1422	C	LEU	1630	11.833	-2.434	19.829	1.00 28.29
MOTA	1423	0	LEU	1630	11.666	-3.412	19.092	1.00 28.56
ATOM	1424	N	VAL	1631	11.933	-2.542	21.150	1.00 29.46
ATOM	1426	CA	VAL	1631	11.883	-3.831	21.833	1.00 29.40
MOTA	1427	CB	VAL	1631	13.222	-4.105	22.553	1.00 27.48
ATOM	1428	CG1	VAL	1631	13.210	-5.477	23.233	1.00 24.53
MOTA	1429	€G2	VAL	1631	14.376	-3.976	21.576	1.00 22.55
MOTA	1430	C	VAL	1631	10.730	-3.918	22.853	1.00 31.94
MOTA	1431	o	VAL	1631	10.630	-3.102	23.787	1.00 33.13
ATOM	1432	N	THR	1632	9.866	-4.911	22.659	1.00 32.21
ATOM	1434	CA	'l'HR	1632	8.728	-5.149	23.540	1.00 31.77
ATOM	1435	CB	THR	1632	7.674	-6.061	22.374	1.00 32.38
MOTA	1436	OG1	THR	1632	8.169	-7.406	22.792	1.00 32.38
ATOM	1438	CG2	THR	1632	7.330	5.554	21.480	1.00 28.05
ATOM	1439	C	THR	1632	9.157	-5.810	24.842	1.00 30.39
ATOM	1440	O	THR	1632	10.256	-6.320	24.947	1.00 30.28
ATOM	1441	N	GLU	1633	8.260	-5.823	25.822	1.00 32.43
MOTA	1443	CA	GLU	1633	8.513	-6.424	27.122	1.00 32.84
MOTA	3.444	CB	GLU	1633	7.259	-6.310	27.991	1.00 35.28
MOTA	1.445	CG	GLU	1633	7.386	-6.881	29.399	1.00 46.57
ATOM	1446	CD	GLU	1633	8.463	-6.192	30.260	1.00 54.03
ATOM	1447	OE1	GLU	1633	8.519	-4.939	30.297	1.00 58.68
MOTA	1448	OE2	GLU	1633	9.249	-6.916	30.918	1.00 56.84
MOTA	1449	C	GLU	1633	8.914	-7.889	26.986	1.00 35.14
MOTA	1450	0	GLU	1633	9.632	-8.435	27.826	1.00 33.92
ATOM	1451	N	ASP	1634	8.456	-8.526	25.910	1.00 38.25
ATOM	1453	CA	ASP	1634	8.768	-9.941	25.677	1.00 39.22
ATOM	1454	CB	ASP	1634	7.588	-10.639	24.990	1.00 44.88
MOTA	1455	CG	ASP	1634	6.258	-10.420	25.725	1.00 54.17
MOTA	1456	OD1	ASP	1634	6.064	-11.042	26.799	1.00 56.33
ATOM	1457	OD2		1634	5.412	-9.622	25.236	1.00 54.47
ATOM	1458	С	ASP	1634		-10.109	24.849	1.00 37.53
ATOM	1459	0	ASP	1634		-11.225	24.495	1.00 36.33
MOTA	1460	N	ASN	1635	10.730	-8.998	24.589	1.00 39.12
ATOM	1462	CA	ASN	1635	11.974	-8.948	23.792	1.00 37.21
ATOM	1463	CB	ASN	1635	13.042	-9.891	24.361	1.00 37.83
ATOM	1464	CG	ASN	1635	13.576	-9.426	25.677	1.00 38.65
ATOM	1465	OD1		1635	13.795	-8.236	25.880	1.00 43.82
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AT		ND2	ASN 1635	13 7	60 10 -		
AT			ASN 1635	11.80	68 -10.3	_	- • • • • • • • • •
ATO	-	0 7	ASN 1635	12.64			87 1.00 35.03
ATO			AL 1636	10.70			48 1.00 32.37
ATC			'AL 1636				36 1.00 33.30
ATC		CB V	AL 1636	10.41			20 1.00 30.50
ATO		CG1 V	AL 1636	8.89 8.60			75 1.00 31.54
ATO		CG2 V	AL 1636	8.38	,	-	34 1.00 29.16
ATO		C V	AL 1636	10.90		_	8 1.00 34.29
ATO		0 V	AL 1636	10.55			9 1.00 29.28
ATO		N M	ET 1637	11.76		_	7 1.00 27.08
ATO		CA MI	ET 1637	12.31	_		3 1.00 27.82
ATO	_	CB MI		13.57	_		4 1.00 27.09
ATOM		CG ME		14.648			7 1.00 27.47
ATON		SD ME		15.243			0 1.00 28.35
ATOM		CE ME		15.243			7 1.00 30.41
ATOM		C ME		11.272			3 1.00 26.00
ATOM	,	O ME		10.751			1.00 26.01
ATOM		N LY		10.751		_	1.00 26.05
ATOM		CA LY		9.984			
ATOM		CB LY		8.693			1.00 22.01
ATOM		CG LY:		7.887			1.00 19.65
ATOM		CD LYS		6.666	-5.254		
ATOM	1494	CE LYS		5.776	4.904	17.869	/ .)
ATOM		NZ LYS		4.970	-6.133	18.076	1.00 19 32
ATOM		C LYS	1638	10.477	-5.522 -3.106	16.869	1.00 23.14
ATOM		O LYS	1638	10.896	-2.147	15.191	1.00 21.85
MOTA MOTA		N ILE	1639	10.371	-3.110	15.808	1.00 24.35
ATOM		CA ILE	1639	10.803	-1.983	13.878	1.00 24.47
ATOM		CB ILE	1639	11.090	-2.443	13.073	1.00 24.90
ATOM		CG2 ILE		11.413	-1.275	11.625	1.00 22.12
ATOM		CG1 ILE	1639	12.256	-3.423	10.720 11.664	1.00 17.41
ATOM		CD1 ILE	1639	12.309	-4.308	10.492	1.00 18.67
ATOM	1508		1639	9.772	-0.856	13.117	1.00 26.15
ATOM	1509 C		1639	8.557	-1.094	12.964	1.00 28.52
ATOM			1640	10.267	0.363	13.358	1.00 27.86
ATOM		A ALA	1640	9.444	1.564	13.445	1.00 30.06
ATOM		B ALA	1640	9.627	2.211	14.812	1.00 29.37
ATOM			1640	9.782	2.566	12.344	1.00 28.25
ATOM			1640	10.808	2.453	11.660	1.00 29.68
ATOM			1641	8.892	3.536	12.154	1.00 30.81
ATOM			1641	9.067		11.154	1.00 30.35
ATOM			1641	10.309	_	11.454	1.00 30.40
ATOM			1641	10.018	<b>-</b> -	12.321	1.00 32.89
ATOM		D1 ASP	1641	10.952			1.00 34.68
ATOM		D2 ASP	1641	8.897			1.00 35.84
ATOM		ASP	1641	9.102	4.162		1.00 38.22
ATOM		ASP	1641	9.484	4.941		1.00 28.91
ATOM		PHE	1642	8.650	2.941		1.00 29.26
ATOM	1527 CA		1642	8.648	2.435		1.00 27.21
ATOM	1528 CB		1642	8.432	0.909		1.00 25.07
	1529 CG	PHE	1642	7.135	0.451		1.00 19.64
						039	1.00 16.47

MOTA	1530	CDI	PHE	1642	5.974	0.400	7.878	1.00	21.72
ATOM	1531	CD2	PHE	1642	7.080	0.018	9.945	1.00	17.01
MOTA	1532	CE	PHE	1642	4.781	-0.082	8.422	1.00	20.97
ATOM	1533	CE2	PHE	1642	5.892	-0.463	10.496	1.00	18.72
ATOM	1534	CZ	PHE	1642	4.743	-0.515	9.739	1.00	20.32
ATOM	1535	С	PHE	1642	7.667	3.174	7.157		25.57
ATOM	1536	0	PHE	1642	7.910	3.292	5.971	1.00	
ATOM	1537	N	GLY	1643	6.585	3.718	7.707		25.69
ATOM	1539	CA	GLY	1643	5.631	4.427	6.866		24.81
MOTA	1540	С	GLY	1643	5.786	5.935	6.893	1.00	
ATOM	1541	0	GLY	1643	4.922	6.684	6.436	1.00	19.20
ATOM	1542	N	LEU	1644	6.930	6.387	7.376		29.50
MOTA	1544	CA	LEU	1644	7.189	7.808	7.491		34.24
ATOM	1545	CB	LEU	1644	8.498	8.037	8.242		33.10
ATOM	1546	CG	LEU	1644	8.473	9.371	8.962	1.00	36.00
ATOM	1547	CD1	LEU	1644	7.520	9.212	10.127		41.52
ATOM	1548		LEU	1644	9.854	9.773	9.442		35.23
ATOM	1549	C	LEU	1644	7.213	8.578	6.179		37.54
ATOM	1550	0	LEU	1644	7.759	8.123	5.176	1.00	
ATOM	1551	N	ALA	1645	6.577	9.744	6.203		41.66
ATOM	1553	CA	ALA	1645	6.524	10.652	5.067	1.00	
ATOM	1554	CB	ALA	1645	5.309	11.563	5.202	1.00	38.13
ATOM	1555	C	ALA	1645	7.819	11.475	5.141	1.00	
ATOM	1556	0	ALA	1645	8.105	12.082	6.176	1.00	
ATOM	1557	N	ALA	1646	8.622	11.462	4.082		45.69
ATOM	1559	CA	ALA	1646	9.871	12.222	4.094	1.00	48.62
ATOM	1560	СВ	ALA	1646	10.971	11.405	4.778		49 50
ATOM	1561	C	ALA	1646	10.338	12.661	2.712		50.98
ATOM	1562	0	ALA	1646	10.319	11.880	1.759	1.00	
ATOM	1563	N	ASP	1647	10.755	13.919	2.598	1.00	53.09
MOTA	1565	CA	ASP	1647	11.253	14.419	1.322	1.00	55.06
ATOM	1566	CB	ASP	1647	10.868	15.887	1.092	1.00	
MOTA	1567	CG	ASP	1647	11.084	16.342	-0.352		59.31
ATOM	1568	OD1	ASP	1647	12.070	15.928	-1.003		59.51
ATOM	1569	OD2	ASP	1647	10.265	17.150	-0.837		63.48
MOTA	1570	С	ASP	1647	12.770	14.264	1.332		55.26
MOTA	1571	0	ASP	1647	13.487	15.075	1.926		53.18
ATOM	1572	N	ILE	1648	13.235	13.198	0.684	1.00	56.66
MOTA	1574	CA	ILE	1648	14.652	12.877	0.595	1.00	57.79
ATOM	1575	CB	ILE	1648	14.890	11.624	-0.271		53.86
ATOM	1576	CG2	ILE	1648	14.133	10.443	0.326	1.00	52.14
MOTA	1577	CG1	ILE	1648	14.454	11.886	-1.718		48.24
MOTA	1578	CD1	ILE	1648	15.198	11.083	-2.751		43.97
ATOM	1579	C	ILE	1648	15.439	14.044	0.014		62.32
ATOM	1580	0	ILE	1648	16.591	14.271	0.380		64.72
MOTA	1581	N	HIS	1649	14.805	14.791	-0.884		65.72
MOTA	1583	CA	HIS	1649	15.450	15.941	-1.500		69.00
ATOM	1584	CB	HIS	1649	14.793	16.285	-2.844		70.35
ATOM	1585	CG	HIS	1649	15.123	15.332	-3.944		73.90
MOTA	1586	CD2	HIS	1649	16.257	14.628	-4.208	1.00	
ATOM	1587		HIS	1649	14.239	15.006	-4.946		75.30
ATOM	1589		HIS	1649	14.798	14.148	-5.779	1.00	
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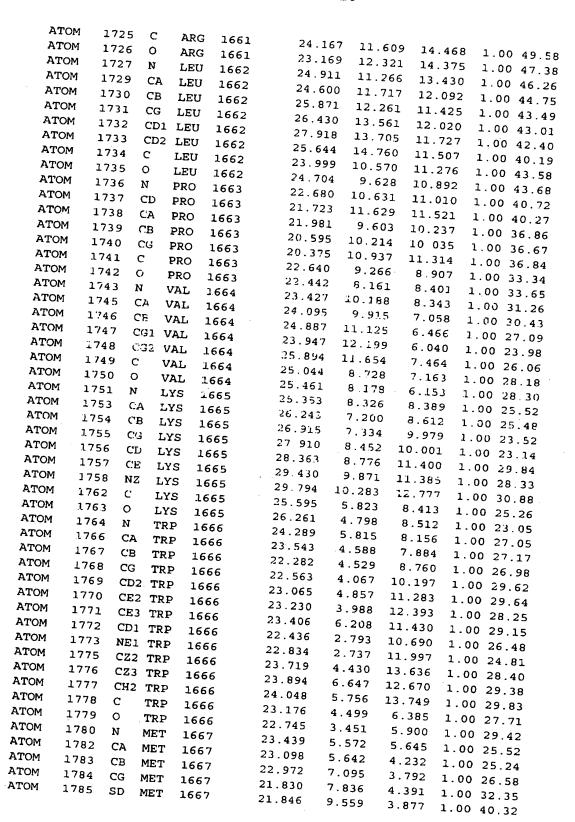
				·
	TOM 159	0 NE2	HIS 1649	
A'	TOM 1592		. •	10.025 13.905 -5 348 1 00 -
A:	TOM 1593			15.419 17.150 -0 576 2 0
	TOM 1594			15.517 18.284 -1 041 1 00
Α٦	rom 1596		-450	15.218 16.912 0 710
AT	TOM 1597			15.199 17.007
AT	OM 1598			13.776 19 400
AT	OM 1599	CD2	HIS 1650	13.272 19 401
AT	OM 1600	MO1 1		13.451 20.724
AT		ND1 I		12,529 19 055
ATO		CE1 F		12.262 10.000
ATO		NE2 F		12.814 21 050
ATO		_	IIS 1650	15.856 17.503
ATC			IS 1650	15.783 18 224 3.029 1.00 71.11
ATC			LE 1651	16 542 35 4-010 1.00 69 56
ATO			LE 1651	17 221 15 3.033 1.00 70.84
ATO			LE 1651	17 622 24 222 1.00 70.50
ATO		CG2 I	LE 1651	4.031 1.00 77 72
ATO	-012	CG1 II	LE 1651	5.194 1 00 21 62
	-413	CD1 II	E 1651	3.890 1 00 22 20
ATO	TOT4	C II		3.593 1 00 75 10
ATON	015	o II		10./34 4.569 1 00 00 00
ATON		N AS		3.745 1 00 70 30
ATOM	~~~0	CA As	P 1652	5.802 1.00 60 00
ATOM	-017	CB AS		19.707 17.987 6.240 1 00 00 05
ATOM	-020	CG AS		7 398 1 (0 70 70
ATOM		OD1 AS	P 1652	20.512 19.790 7.843 1 00.73 26
ATOM	1622 (	DD2 ASI	1652	21.306 20.248 6.985 1 00 73 36
ATOM	1623 (	ASI		20.646 20.034 9.060
ATOM	1624 (	ASE		20.802 17.023 6 672 3 66
ATOM	1625 N			20.746 16.457 7.763
ATOM	1627 C	'A TYR		21.802 16.856 5.814 1 00 54 1
MOTA	1628 C	B TYR		22.926 15.968 6.089 1.06 63.00
MOTA	1629 C	G TYR		23.852 15.906 4 875 1 05
MOTA		D1 TYR		23.362 14.971 3.795 1.00 61.29
ATOM		E1 TYR	- <del>-</del>	24.153 14.679 2 684 1 00 52.37
ATOM		D2 TYR	1653	23.725 13.773 1 717 1 00 61.11
ATOM		E2 TYR	1653	22.121 14.335 3 910 1 00 62.89
MOTA	1634 C2		1653	21.685 13.429 2 952 7 00 64.11
ATOM	1635 OF		1653	22.487 13.148 1 850 1.00 66.09
ATOM	1637 C		1653	22.044 12.239 0.033
ATOM	1638 O		1653	23.733 16.313 7.345
ATOM	1639 N	TYR TYR	1653	24.403 15.453 7.913
ATOM	1641 CA		1654	23.644 17.564 7.700
ATOM	1642 CB		1654	24.379 18 013
ATOM			1654	24.947 10.417
ATOM		TYR	1654	26.038 10.467
ATOM		TYR	1654	25.736 10.600 7.091 1.00 57.70
ATOM		LTYR	1654	26.734 19.700
ATOM		TYR	1654	27.364 10.252 5.383 1.00 60.65
ATOM		TYR	1654	28.366 19.262 8.035 1.00 56.79
ATOM	1648 CZ	TYR	1654	28.047 10.400 7.079 1.00 58.85
h moss	1649 OH		1654	29.048 19.405 5.754 1.00 60.88
01/1	1651 C	TYR	1654	23.560 17 000 4.806 1.00 64.23
				23.560 17.980 10.239 1.00 65.89
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MOTA 1652 0 TYR 1654 18.283 11.316 1.00 67.56 24.074 MOTA 1653 N LYS 1655 22.297 17.586 10.135 1.00 67.36 ATOM 1655 CA LYS 1655 21.443 17.527 11.315 1.00 69.11 ATOM 1656 LYS CB 1655 19.972 17.611 10.915 1.00 69.86 **ATOM** 1657 CG LYS 19.019 12.090 1655 17.651 1.00 71.45 **ATOM** 1658 CD LYS 1655 17.607 17.867 11.603 1.00 75.40 ATOM 1659 CE LYS 1655 16.595 17.393 12.627 1.00 78.22 ATOM 1660 NZLYS 1655 15.204 17.553 12.110 1.00 80.61 MOTA 1664 С LYS 1.655 21.714 16.242 12.093 1.00 69.65 MOTA 1665 0 LYS 1655 21.872 15.169 11.497 1.00.70.67 MOTA 1666 N LYS 1656 21.766 16.358 13.419 1.00 68.19 MOTA 1668 CA LYS 1656 22.035 15.212 14.275 1.00 68.00 ATOM 1669 CB LYS 1656 22.983 15.618 15.403 1.00 65.53 ATOM 1670 CG LYS 1656 24.395 15.895 14.946 1.00 62.71 **ATOM** 1671 CD LYS 1656 25.280 16.221 16.138 1.00 64.38 **ATOM** 1672 CE LYS 1656 26.764 16.031 15.832 1.00 63.23 ATOM 1673 NZ LYS 1656 27.592 16.186 17.062 1.00 61.72 ATOM 1677 C LYS 1656 20.777 14.560 14.855 1.00 68.73 ATOM 1678 LYS О 19.695 14.837 1656 15 148 1.00 69.20 **ATOM** 1679 N THR 1657 20.928 13.337 15.359 1.00 68.48 ATOM 1681 CA THR 1657 19.821 12.607 15.960 1.00 67.93 **ATOM** 1682 CB THR 1657 20.109 11.078 16.021 1.00 68.93 MOTA 1683 OG1 THR 1657 21.295 10.823 16.787 1.00 68.72 ATOM 1685 CG2 THR 10.500 1657 20.289 14.637 1.00 68.83 ATOM 1686 C THR 19.682 1657 13.131 17.383 1.60 67.80 ATOM 1687 THR 20.424 14.022 0 1657 17.790 1.00 67.87 ATOM 1688 N ALA 1658 18.753 12.569 18.148 1.00 68.95 **ATOM** 1690 CA ALA 12.992 1658 18.580 19.537 1.00 70.64 **ATOM** 1691 CB ALA 1658 17.391 12.254 20.173 1.00 71.19 ATOM 12.709 1692 C ALA 1658 19.880 20.313 1.00 69.64 ATOM 1693 0 ALA 1658 20.394 13.566 21.042 1.00 70.13 MOTA. 1694 N ASN 1659 20.440 11.526 20.080 1.00 68.02 **ATOM** 1696 CA ASN 21.663 11.092 1659 20.746 1.00 66.10 ATOM 1697 CB ASN 1659 21.835 9.583 20.557 1.00 70.23 ATOM 1698 CG ASN 1659 22.632 8.937 21.679 1.00 74.09 ATOM 1699 OD1 ASN 1659 22.525 9.331 22.840 1.00 75.21 ATOM 1700 ND2 ASN 1659 23.402 7.907 21.342 1.00 75.03 **ATOM** 1703 C ASN 1659 22.910 11.816 20.249 1.00 63.30 MOTA 1704 0 ASN 24.004 1659 11.585 20.762 1.00 61.12 MOTA 1705 N GLY 1660 22.744 12.678 19.246 1.00 61.61 ATOM 1707 CA GLY 1660 23.867 13.421 18.689 1.00 59.06 ATOM 1708 С GLY 1660 24.604 12.750 17.536 1.00 56.84 ATOM 1709 0 GLY 1660 25.726 13.132 17.196 1.00 55.69 MOTA 1710 N ARG 1661 23.980 11.758 16.914 1.00 55.73 MOTA 1712 CA ARG 1661 24.626 11.062 15.808 1.00 52.76 **ATOM** 1713 CB ARG 1661 24.387 9.549 15.883 1.00 52.39 ATOM 1714 CG ARG 1661 24.977 8.874 17.111 1.00 54.08 ATOM 1715 ARG CD 1661 24.776 7.376 17.045 1.00 58.37 MOTA 1716 NE ARG 1661 25.178 6.665 18.260 1.00 59.27 ATOM 1718 CZARG 1661 24.952 5.369 18.471 1.00 59.83 ATOM 1719 NH1 ARG 1661 4.643 24.319 17.550 1.00 57.04 **ATOM** 1722 NH2 ARG 1661 25.375 4.792 19.591 1.00 59.47



ATOM	1786	CE	MET	1667	21.033	9.447	2.341	1.00 38.17
ATOM	1787	С	MET	1667	24.042	4.960	3.276	1.00 25.07
ATOM	1788	0	MET	1667	25.256	5.037	3.411	1.00 27.61
ATOM	1789	N	ALA	1668	23.473	4.302	2.282	1.00 24.92
ATOM	1791	CA	ALA	1668	24.272	3.647	1.271	1.00 26.92
ATOM	1792	CB	ALA	1668	23.397	2.720	0.425	1.00 25.09
ATOM	1793	C	ALA	1668	24.866	4.759	0.410	1.00 27.82
MOTA	1794	0	ALA	1668	24.254	5.817	0.242	1.00 27.06
ATOM	1795	N	PRO	1669	26.050	4.530	-0.170	1.00 27.84
ATOM	1796	CD	PRO	1669	26.912	3.339	-0.107	1.00 27.12
ATOM	1797	CA	PRO	1669	26.662	5.561	-1.005	1.00 28.04
MOTA	1798	CB	PRO	1669	27.868	4.835	-1.593	1.00 26.71
ATOM	1799	CG	PRO	1669	28.249	3.893	-0.498	1.00 27.49
ATOM	1800	C	PRO	1669	25.734	6.078	-2.108	1.00 28.51
ATOM	1801	0	PRO	1669	25.685	7.281	-2.371	1.00 30.64
ATOM	1802	N	GLU	1670	24.992	5.179	-2.746	1.00 28.25
ATOM	1804	CA	GLU	1670	24.095	5.584	-3.826	1.00 26.82
ATOM	1805	CB	GLU	1670	23.600	4.369	-4.620	1.00 29.32
MOTA	1806	CG	GLU	1670	22.604	3.486	-3.889	1.00 30.38
MOTA	1807	CD	GLU	1670	23.223	2.266	-3.229	1.00 32.52
MOTA	1808	OE1		1670	22.444	1.393	-2.794	1.00 28.06
MOTA	1809	OE2	GLU	1670	24.474	2.175	-3.130	1.00 28.67
MOTA	1810	C	GLU	1670	22.924	6.440	-3.356	1.00 24.79
ATOM	1811	0	GLU	1670	22.410	7.236	-4.123	1.00 22.31
MOTA	1812	N	ALA	1671	22.512	6.265	-2.101	1.00 26.70
ATOM	1814	CA	ALA	1671	21.423	7.040	-1.490	1.00 25.67
MOTA	1815	CB	ALA	1671	20.813	6.292	-0.312	1.00 18.88
MOT'A	1816	C	ALA	1671	21.984	8.365	-1.006	1.00 26.05
ATOM	1817	0	ALA	1671	21.400	9.414	-1.229	1.00 28.14
ATOM	1818	N	LEU	1672	23.138	8.300	-0.358	1.00 29.03
ATOM	1820	CA	LEU	1672	23.807	9.481	0.172	1.00 34.07
ATOM	1821	CB	LEU	1672	25.030	9.064	0.986	1.00 34.45
ATOM	1822	CG	LEU	1672	25.870	10.157	1.648	1.00 39.50
ATOM	1823		LEU	1672	25.081	10.853	2.740	1.00 41.71
MOTA	1824		LEU	1672	27.123	9.530	2.243	1.00 40.16
ATOM	1825	С	LEU	1672	24.248	10.431	-0.942	1.00 38.47
ATOM	1826	0	LEU	1672	23.958	11.625	-0.898	1.00 42.25
ATOM	1827	N	PHE	1673	24.924	9.901	-1.956	1.00 39.07
ATOM	1829	CA	PHE	1673	25.414	10.725	-3.053	1.00 38.00
ATOM	1830	СВ	PHE	1673	26.699	10.110	-3.639	1.00 36.48
ATOM	1831	CG	PHE	1673	27.826	9.928	-2.637	1.00 33.36
ATOM	1832		PHE	1673	28.524	8.724	-2.580	1.00 29.55
ATOM	1833		PHE	1673	28.205	10.960	-1.779	1.00 31.85
ATOM	1834		PHE	1673	29.580	8.540	-1.692	1.00 26.33
ATOM	1835		PHE	1673	29.265	10.786	-0.880	1.00 30.95
ATOM	1836	CZ	PHE	1673	29.954	9.568	-0.838	1.00 28.99
ATOM	1837	С	PHE	1673	24.413	10.957	-4.194	1.00 39.64
ATOM	1838	0	PHE	1673	24.364	12.046	-4.760	1.00 37.72
ATOM	1839	N	ASP	1674	23.651	9.928	-4.554	1.00 41.35
ATOM	1841	CA	ASP	1674	22.716	10.027	-5.666	1.00 43.38
ATOM	1842	CB	ASP	1674	22.934	8.858	-6.625	1.00 47.84
MOTA	1843	CG	ASP	1674	24.359	8.765	-7.121	1.00 53.24

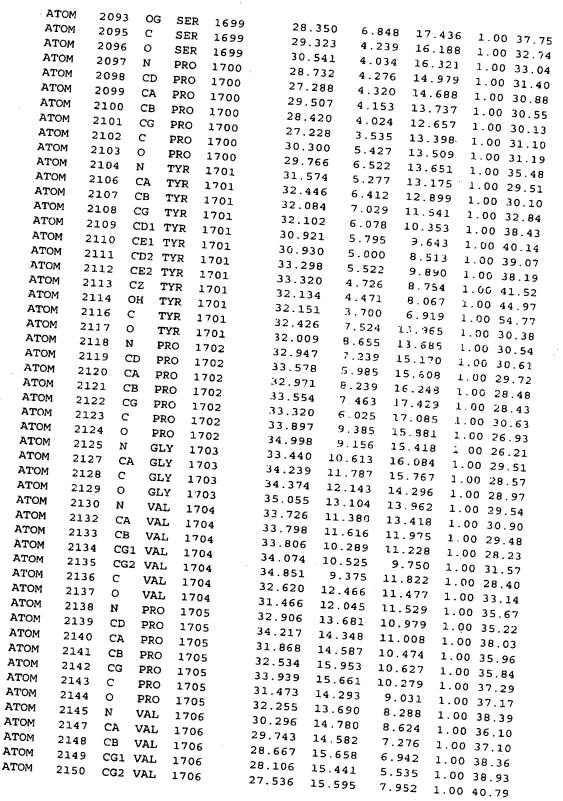
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	TOM 1844			25.	040 0		
	TOM 1845	OD2 ASP	1674	24.		808 -7.1	
	OM 1846	C ASP				640 -7.4	60 1.00 55.73
	OM 1847	O ASP		21.5		_	21 1.00 45.94
	OM 1848	N ARG	1675	20.4			22 1.00 47.80
	OM 1850	CA ARG	1675	20.9		953 -4.0	40 1.00 45.98
AT		CB ARG	1675	19.5		981 -3.60	
AT		CG ARG	1675	18.8		346 -3.88	
ATO		CD ARG		19.5		78 -3.14	
ATO	OM 1854	NE ARG	1675	19.4		15 -3.99	
ATO	DM 1856	CZ ARG	1675	20.0		67 -3.30	
ATC		NH1 ARG	1675	19.6		16 -3.47	
ATC		NH2 ARG	1675	18.6	10 16.3		
ATO			1675	20.19	94 17.0		4- 42.00
ATO		-410	1675	18.64	7 8.8		07,42
ATO			1675	17.46	9.0		
ATO			1676	19.27	0 7.74		
ATO		CA ILE	1676	18.54	4 6.61		
ATO	M 3055	CB ILE	1676	19.32			,0
ATO	4	CG2 ILE	1676	1.8.45			,
ATON		CG1 ILE	1676	19.76		-	
ATOM			1676	20.65			00
ATOM	-0,2	CILE	1676	18.32		-	
ATOM	1075		1676	19.26			51.00
ATOM	1074 1		1677	17.102			- ~0.7/
ATOM	10		1677	16.779			1.00 30.32
ATOM			1677	15.846			1.00 29.68
ATOM		G TYR	1677	16.523			1.00 31.14
ATOM		D1 TYR	1677	16.616			1 00 32.95
		E1 TYR 1	677	17.208			1.00 30.40
ATOM		D2 TYR 1	.677	17.048			1.00 27.57
ATOM		E2 TYR 1	677	17.642			1.00 32.13
ATOM	1883 C	Z TYR 1	677	17.711	7.059		1.00 31.50
ATOM	1884 O	· ·	677	18.235	8.366	1.081	1.00 31.12
ATOM	1886 C		677	16.123	9.326	1.912	1.00 32.18
ATOM	1887 O		677	15.268	3,424	-2.933	1.00 28.88
ATOM	1888 N	~~~	678	16.556	3.537	-3.811	1.00 32.20
ATOM	1890 C		578		2.253	-2.481	1.00 26.34
ATOM	1891 CE		578	16.023	0.988	-2.971	1.00 25.55
ATOM	1892 OG		578	16.917	0.394	-4.043	1.00 28.81
ATOM	1894 CG	_	78	18.221	0.179	-3.483	1.00 34.06
ATOM	1895 C		78	17.010	1.320	-5.267	1.00 27.25
ATOM	1896 O		78	16.037	0.007	-1.827	1.00 21.78
ATOM	1897 N		79	16.505	0.312		1.00 25.57
ATOM	1899 CA		79 79	15.559	~1.198		1.00 20.86
ATOM	1900 CB			15.580	-2.216		1.00 20.30
ATOM	1901 CG			14.816	-3.453		1.00 17.22
MOTA				13.367	-3.196		1.00 17.22
ATOM				12.662	-3.275		1.00 19.02
ATOM				12.459	-2.830		1.00 14.89
ATOM				11.260	-2.697		1 00 16
ATOM	1908 C			11.359	-2.961		1.00 16.10
ATOM	1909 O	HIS 167		17.050	_		.00 15.18
	=200	HIS 167	9		-2.901		.00 20.44
						J.JJ6 1	.00 22.58

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MOTA	1910	N	GLN	1680	17.874	-2.310	-1.781	1.00 20.58
ATOM	1912	CA	GLN	1680	19.303	-2.539	-1.721	1.00 22.70
ATOM	1913	CB	GLN	1680	19.935	-2.427	-3.106	1.00 26.26
ATOM	1914	CG	GLN	1680	19.934	-3.711	-3.889	1.00 31.86
MOTA	1915	CD	GLN	1680	18.949	-3.687	-5.026	1.00 37.54
MOTA	1916	OE1	GLN	1680	17.931	-3.000	-4.961	1.00 42.70
ATOM	1917	NE2	GLN	1680	19.256	-4.409	··6.091	1.00 37.42
MOTA	1920	С	GLN	1680	19.985	-1.559	-0.797	1.00 24.93
ATOM	1921	0	GLN	1680	20.875	-1.943	-0.039	1.00 26.39
MOTA	1922	N	SER	1681	19.605	-0.286	-0.867	1.00 24.70
MOTA	1924	CA	SER	1681	20.239	0.678	0.030	1.00 23.24
MOTA	1925	CB	SER	1681	19.923	2.128	-0.346	1.00 19.33
ATOM	1926	OG	SER	1681	18.544	2.326	-0.545	1.00 18.55
MOTA	1928	C	SER	1681	19.852	0.364	1.464	1.00 21.77
ATOM	1929	0	SER	1681	20.645	0.609	2.366	1.00 24.14
ATOM	1930	N	ASP	1682	18.659	-0.210	1.670	1.00 21.80
MOTA	1932	CA	ASP	1682	18.180	-0.604	3.003	1.00 22.45
ATOM	1933	CB	ASP	1682	16.730	-1.111	2.963	1.00 25.27
MOTA	1934	CG	ASP	1682	15.678	0.004	3.132	1.00 28.21
ATOM	1935	OD1	ASP	1682	14.500	0.245	2.786	1.00 25.41
ATOM	1936	OD2	ASP	1682	15.992	1.102	3.639	1.00 30.19
ATOM	1937	С	ASP	1682	19.076	-1.736	3.517	1.00 23.69
ATOM	1.938	O	ASP	1682	19.385	-1.799	4.709	1.00 24.74
ATOM	1939	11	VAL	1683	19.474	-2.635	2.620	1.00 23.49
ATOM	1941	CA	VAL	1683	20.354	-3.737	3.003	1.00 21.77
ATOM	1942	CB	VAL	1683	20.543	-4.741	1.837	1.00 20.49
MOTA	1943		VAL	1683	21.770	5.613	2.039	1 00 19.82
ATOM	1944		VAL	1683	19.320	-5.618	1.736	1.00 19.29
MOTA	1945	C	.IAV	1683	21.674	-3.153	3.523	1.00 21.93
ATOM	1946	Ó	VAL	1683	22.161	-3.570	4.573	1.00 21.06
ATOM	1947	N	TRP	1684	22.207	-2.143	2.837	1.00 20.64
ATOM	1949	CA	TRP	1684	23.424	-1.482	3.295	1.00 20.98
ATOM	1950	СВ	TRP	1684	23.711	-0.224	2.463	1.00 19.56
ATOM	1951	CG	TRP	1684	24.859	0.609	2.970	1.00 23.22
ATOM	1952	CD2	TRP	1684	26.182	0.686	2.421	1.00 24.64
ATOM	1953	CE2	TRP	1684	26.929	1.559	3.249	1.00 24.69
ATOM	1954	CE3	TRP	1684	26.813	0.102	1.315	1.00 26.41
A'TOM	1955	CD1	TRP	1684	24.857	1.430	4.075	1.00 23.64
ATOM	1956	NE1		1684	26.097	1.994	4.246	1.00 23.28
ATOM	1958		TRP	1684	28.275	1.859	3.000	1.00 20.55
ATOM	1959	CZ3	TRP	1684	28.165	0.409	1.072	1.00 20.33
ATOM	1960	CH2	TRP	1684	28.872	1.274	1.908	1.00 22.82
ATOM	1961	C	TRP	1684	23.201	-1.112	4.771	1.00 13.24
ATOM	1962	0	TRP	1684	23.931	-1.560	5.652	1.00 21.12
MOTA	1963	N	SER	1685		-0.342		
ATOM	1965	CA	SER	1685	22.150		5.032	1.00 23.27
ATOM	1966	CB	SER		21.787	0.086	6.386	1.00 22.54
ATOM	1966			1685	20.429	0.768	6.356	1.00 21.98
ATOM		OG C	SER	1685	20.318	1.626	5.220	1.00 25.48
	1969	C	SER	1685	21.747	-1.068	7.389	1.00 21.33
ATOM	1970	0	SER	1685	22.145	-0.902	8.545	1.00 19.52
ATOM	1971	N	PHE	1686	21.260	-2.228	6.946	1.00 23.10
ATOM	1973	CA	PHE	1686	21.174	-3.424	7.800	1.00 23.09

λπ	OM 1974			
		CB PH		20.409 -4.550 7.095 1.00 22 77
AT		CG PHI		20 102 5 77
	-2,0	CD1 PHE		19 370 5 501
AT		CD2 PHE		20 809 6 200
AT		CE1 PHE	1686	19 185 6 000
ATO		CE2 PHE	1686	20 622 2 100 24.25
ATO		CZ PHE		8.455 1.00 22 67
ATO		C PHE	1686	9.585 1.00 26 30
ATC		O PHE	1686	22.309 -3.919 8.240 1.00 21 77
ATC	M 1983	N GLY	1687	22.739 -4.450 9.350 1.00 20 47
ATO	M 1985	CA GLY	1687	23.553 -3.773 7.358 1.00 20 63
ATO	M 1986	C GLY	1687	7.685 1.00 19 20
ATO		O GLY	1687	23.407 ~3.276 8.822 1.00 21 64
ATO	M 1988	N VAL	1688	26.094 -3.755 9.727 1.00 19.46
ATO		CA VAL		25.008 -1.996 8.794 7.00 22 10
ATO		CB VAL	1688	25.372 ~1.024 9.831 1.00 21.22
ATO			1688	25.048 0.458 9.423 1.00 22.05
ATON	_	CG1 VAL CG2 VAL	1688	25.439 1.424 10.540 1.00 23.20
ATOM		_	1688	25 920
ATOM	1	C VAL	1688	24 621 1 400 = 100 24,23
ATOM		O VAL	1688	25 204 1 465
ATOM		I LEU	1689	23 339 1 72
ATOM		CA LEU	1689	22 542 2 25
ATOM		B LEU	1689	21 072 2 202
ATOM		G LEU	1689	19 901 2 425
ATOM		D1 LEU	1689	18 514 2 22
ATOM		D2 LEU	1689	20 049 2 702
ATOM	2003 C	LEU	1689	23 150 2 445
	2004 O	LEU	1689	23 202 2 702
ATOM	2005 N	LEU	1690	23 514 4 255
ATOM	2007 C	A LEU	1690	24 255 5 501
ATOM	2008 C	B LEU	1690	24 770 6 55
ATOM	3000 G		1690	23 800 7 500
ATOM		D1 LEU	1690	24 662 0 050
ATOM	2011 CI	D2 LEU	1690	22 22 1.00 25.45
ATOM	2012 C		.690	25 1.00 21.17
ATOM	2013 O		690	25.471 -5.204 13.189 1.00 26.51
ATOM	2014 N		691	26.710 -5.747 14.273 1.00 29.07
MOTA	2016 CA	-	691	27 455 12.660 1.00 26.26
MOTA	2017 CB		691	3.761 13.341 1.00 25 08
MOTA	2018 CG		691	20.129 -2.706 12.493 1.00 25 16
ATOM		~	691	23.436 24.268 13.039 1.00 27 40
ATOM	2020 CE	_	691	23.701 -1.163 13.925 1.00 25 81
ATOM		<b>-</b>		34.100 -1.070 14.103 1.00 22 62
ATOM			591 501	28.870 -0.236 14.575 1.00 26 70
ATOM			591	30.688 -2.798 12.735 1.00 23.02
ATOM	2025 CZ2		591	31.675 -2.078 13.371 1.00 25 45
ATOM			91	31.690 -0.085 14.900 3.00 32.55
ATOM			91	29.459 0.745 15.371 1.00 25 65
ATOM			91	30 061 0 0
ATOM			91	27 114 2 2 2 2 2 3 1 2 3 2 3 2 3 2 3 2 3 2 3 2
ATOM	000		91	27 971 2 225
ATOM	2030 N	GLU 16	92	25 995 2 73
014	2032 CA	GLU 16	92	25 574
				23.374 -1.938 16.155 1.00 24.98

ATOM	2033	CB	GLU	1692	24.335	-1.060	15.994	1.00 22.29
ATOM	2034	CG	GLU	1692	24.507	0.107	15.056	1.00 18.31
MOTA	2035	CD	GLU	1692	23.255	0.933	14.978	1.00 25.10
MOTA	2036	OE1	GLU	1692	22 433	0.704	14.066	1.00 26.95
MOTA	2037	OE2	GLU	1692	23.067	1.815	15.840	1.00 27.05
ATOM	2038	С	GLU	1692	25.260	-3.036	17.163	1.00 25.18
ATOM	2039	0	GLU	1692	25.602	-2.927	18.341	1.00 26.12
MOTA	2040	N	ILE	1693	24.593	-4.087	16.698	1.00 27.16
MOTA	2042	CA	ILE	1693	24.231	-5.214	17.555	1.00 25.91
MOTA	2043	CB	ILE	1693	23.373	-6.287	16.777	1.00 25.70
ATOM	2044	CG2	ILE	1693	23.171	-7.564	17.638	1.00 18.73
MOTA	2045	CG1	ILE	1693	22.005	-5.682	16.382	1.00 23.45
MOTA	2046	CD1	ILE	1693	21.208	-6.485	15.346	1.00 15.62
ATOM	2047	C	ILE	1693	25.496	-5.847	18.107	1.00 26.70
MOTA	2048	0	ILE	1693	25.672	-5.961	19.316	1.00 28.19
ATOM	2049	N	PHE	1694	26.442	-6.133	17.229	1.00 28.78
MOTA	2051	CA	PHE	1694	27.664	-6.779	17.679	1.00 29.72
MOTA	2052	CB	PHE	1694	28.261	-7.598	16.542	1.00 27.18
MOTA	2053	CG	PHE	1694	27.315	-8.649	16.048	1.00 25.38
ATOM	2054	CDi	PHE	1694	26.793	-8.599	14.770	1.00 26.16
ATOM	2055	CD2	PHE	1694	26.844	-9.625	16.919	1.00 26.37
ATOM	2056	CE1	PHE	1694.	25.808	-9.505	14.370	1.00 31.37
ATOM	2057	CE2	PHE	1694	25.863	-10.533	16.536	1.00 25.23
MOTA	2058	CZ	PHE	1694		-10.478	15.268	1.00 29.46
MOTA	2059	С	PHE	1694	28.663	-5.906	18 438	1.00 30.92
MOTA	2060	0	PHE	1694	29.697	-6.403	18.902	1.00 32.23
ATOM	5061	N	THR	1695	28.344	-4.616	18.575	1.00 29 46
MOTA	2063	CA	THR	1695	29.170	-3.698	19.348	1.00 27.17
ATOM	2064	CB	THR	1695	29.665	-2.474	18.535	1.00 23.32
ATOM	2065	OG1	THR	1695	28.553	-1.710	18.046	1.00 24.73
ATOM	2067	CG2	THR	1695	30.538	-2.914	17.395	1.00 21.34
ATOM	2068	C	THR	1695	28.307	-3.230	20.519	1.00 28.81
ATOM	2069	0	THR	1695	28.707	-2.346	21.289	1.00 31.85
ATOM	2070	N	LEU	1696	27.130	-3.841	20.651	1.00 26.30
ATOM	2072	CA	LEU	1696	26.188	-3.523	21.720	1.00 25.99
MOTA	2073	CB	LEU	1696	26.704	-4.043	23.060	1.00 24.51
ATOM	2074	CG	LEU	1696	26.974	-5.539	23.194	1.00 23.32
MOTA	2075	CD1	LEU	1696	27.447	-5.843	24.597	1.00 26.45
ATOM	2076	CD2	LEU	1696	25.726	-6.297	22.907	1.00 29.79
ATOM	2077	С	LEU	1696	25.892	-2.036	21.837	1.00 24.90
ATOM	2078	0	LEU	1696	26.083	-1.457	22.889	1.00 28.99
ATOM	2079	N	GLY	1697	25.386	-1.432	20.771	1.00 25.05
MOTA	2081	CA	GLY	1697	25.072	-0.016	20.811	1.00 24.31
ATOM	2082	С	GLY	1697	26.241	0.847	20.381	1.00 27.15
ATOM	2083	0	GLY	1697	26.297	2.035	20.701	1.00 29.57
MOTA	2084	N	GLY	1698	27.177	0.261	19.639	1.00 27.33
ATOM	2086	CA	GLY	1698	28.319	1.023	19.178	1.00 27.04
ATOM	2087	C	GLY	1698	27.966	2.109	18.173	1.00 29.78
ATOM	2088	0	GLY	1698	27.115	1.929	17.301	1.00 32.03
ATOM	2089	N	SER	1699	28.633	3.247	18.295	1.00 32.03
ATOM	2091	CA	SER	1699	28.413	4.385	17.414	1.00 30.60
ATOM	2092	CB	SER	1699	28.747	5.692	18.164	1.00 31.48
			~		20.737	3.032	+0.104	1.00 32.37



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ATOM	2151	С	VAL	1706	30.762	14.559	6.138	1.00	37.09
ATOM	2152	0	VAL	1706	30.927	13.543	5.461	1.00	38.75
ATOM	2153	N	GLU	1707	31.477	15.663	5.967	1.00	37.08
ATOM	2155	CA	GLU	1707	32.472	15.793	4.910	1.00	35.52
ATOM	2156	CB	GLU	1707	33.059	17.206	4.918	1.00	38.30
ATOM	2157	C	GLU	1707	33.588	14.762	4.945	1.00	34.20
ATOM	2158	0	GLU	1707	34.153	14.445	3.908	1.00	33.48
MOTA	2159	N	GLU	1708	33.936	14.273	6.132	1.00	34.20
. ATOM	2161	CA	GLU	1708	34.981	13.256	6.241	1.00	36.08
MOTA	2162	CB	GLU	1708	35.555	13.178	7.660	1.00	40.39
MOTA	2163	CG	GLU	1708	36.212	14.464	8.179	1.00	45.41
MOTA	2164	CD	GLU	1708	37.471	14.871	7.430	1.00	50.66
ATOM	2165	OE1	GLU	1708	38.199	13.986	6.909	1.00	54.73
ATOM	2166	OE2	GLU	1708	37.747	16.092	7.392	1.00	52.85
MOTA	2167	C	GLU	1708	34.369	11.911	5.855	1.00	35.22
ATOM	2168	0	GLU	1708	35.035	11.045	5.260	1.00	34.04
ATOM	2169	N	LEU	1709	33.089	11.749	6.178	1.00	33.30
MOTA	2171	CA	LEU	1709	32.376	10.519	5.860	1.00	31.44
ATOM	2172	CB	LEU	1709	30.975	10.531	6.474	1.00	26.89
ATOM	2173	CG	LEU	1709	30.065	9.366	6.073	1.00	26.05
MOTA	2174	CD1	LEU	1709	30.652	છ.036	6.503	1.00	22.75
ATOM	2175	CD2	LEU	1709	28.717	9.574	6.537	1.00	26.15
ATOM	2176	C	LEU	1709	32.291	10.325	4.350	1.00	31.18
ATOM	2177	O	LEU	1709	32.490	9.209	3.856	1.60	29.88
ATOM	2178	N	PHE	1710	32.011	11.408	3.623	1.00	30.16
ATOM	2180	CA	PHE	1710	31.915	11.333	2.169	1.00	31.64
ATOM	2181	CB	PHE	1710	31.658	12.710	1.567	1.00	33.44
ATOM	2182	CG	PHE	1710	30.287	13.231	1.827	1.00	37.78
ATOM	2183	CD1	PHE	1710	29.287	12.395	2.303	1.00	41.46
ATOM	2184	CD2	PHE	1710	29.991	14.565	1.613	1.00	40.72
ATOM	2185	CE1	PHE	1710	28.012	12.882	2.566	1.00	41.30
ATOM	2186	CE2	PHE	1710	28.715	15.058	1.875	1.00	42.99
ATOM	2187	CZ	PHE	1710	27.725	14.208	2.354	1.00	4C.95
ATOM	2188	C	PHE	1710	33.202	10.771	1.609	1.00	32.38
MOTA	2189	O	PHE	1710	33.183	9.815	0.825	1.00	32.26
MOTA	2190	N	LYS	1711	34.310	11.336	2.085	1.00	31.26
MOTA	2192	CA	LYS	1711	35.664	10.971	1.697	1.00	29.73
MOTA	2193	CB	LYS	1711	36.642	11.932	2.379		33.49
MOTA	2194	CG	LYS	1711	38.103	11.716	2.042	1.00	39.79
MOTA	2195	CD	LYS	1711	38.981	12.731	2.755	1.00	43.35
MOTA	2196	CE	LYS	1711	40.413	12.686	2.238	1.00	4€.23
MOTA	2197	NZ	LYS	1711	41.116	11.422	2.600	1.00	53.67
ATOM	2201	С	LYS	1711	35.999	9.501	2.015	1.00	29.34
ATOM	2202	0	LYS	1711	36.670	8.836	1.231	1.00	28.77
ATOM	2203	N	LEU	1712	35.541	9.000	3.164	1.00	30.40
ATOM	2205	CA	LEU	1712	35.776	7.599	3.532	1.00	28.72
ATOM	2206	CB	LEU	1712	35.241	7.295	4.942		27.71
ATOM	2207	CG	LEU	1712	35.971	7.870	6.166	1.00	28.23
ATOM	2208	CD1	LEU	1712	35.186	7.593	7.440	1.00	20.80
ATOM	2209	CD2	LEU	1712	37.389	7.297	6.266	1.00	27.01
MOTA	2210	C	LEU	1712	35.022	6.738	2.530	1.00	30.03
ATOM	2211	0	LEU	1712	35.571	5.796	1.957	1.00	29.28

	TOM 2212	N LEU 171	
	rom 2214	CA LEU 171	2.325 1 00 31 00
	rom 2215	CB LEU 171:	0.339 1.403 1.00 74 30
	TOM 2216		31.467 6.872 1.447 1.00 37.65
	OM 2217	CD1 LEU 1713	30.663 6.450 2.686 7.00 ==
	OM 2218	CD2 LEU 1713	29.367 7.217 2 781 1 20 37.08
AT	OM 2219	C LEU 1713	30.399 4.950 2.641 1.00 37.03
AT	OM 2220	O LEU 1713	33.451 6.344 -0.011 1.00 3-
AT	OM 2221		33.468 5.298 -0.662 1.00 35.45
ATO	OM 2223	CD 1/14	33.920 7.498 -0.481 1.00 38.18
ATO	OM 2224	1,14	34.487 7.590 -1.821 1.00 33.22
ATO	DM 2225	7714	34.881 9.027 -2 150 1 22
ATO		CD ****	33.724 9.962 -2 390 1 22
ATO	M 2227	00 1/14	32.814 9.439 -3.491 1.00 -3
ATO		I/14	31.613 10.364 -3 720 1 00 39.40
ATO	M 2232	0	30.674 9.841 -4 771 1.00 74
ATO	M 2233	0	35 706 6 670
ATO	M 22-	210 1/14	35 998 2.00 32.53
ATO	M 222	020 1/15	36,420 6,400
ATO	M 222	CD	37.602 5.644 -0.864 1.00 33.50
ATOM		720 1/15	38 617 6 177
ATOM	4 2000	CD	39 085 7 500
ATOM	1	000	39.654 9.370
ATOM			39.820 7.826 2.065 1.00 51.44
ATOM		1/13	39.930 0.573
ATOM		220 1/15	37 278 4 202
ATOM	=	_ 020 1,15	38.184 3 357 0 150 1.00 35.09
ATOM			35.991 3 966 3 1.00 37.59
ATOM	2247 C	771 1/10	35.576 2.499 3.79
ATOM	2248 0	1/10	35.852
ATOM	2249 N	1/10	35 906 0 766 21.00 29.06
ATOM	2251 C	2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2	35 995 3 975
ATOM	2252 CI	111/	36 292
ATOM	2253 C		36 534 2 745 = 2.00 29.80
ATOM		1/1/	36 794 3 460
ATOM		D2 HIS 1717	37 955
ATOM		01 HIS 1717	35.782 3.279 6.746 1.00 35.38
ATOM		E1 HIS 1717 E2 HIS 1717	36.309 3.000 5.00 37.81
ATOM	2260 C		37.624 3 134
ATOM	2261 0	HIS 1717	35 171 1 645
ATOM	2262 N	HIS 1717	33.987 1.900 3.940 1.00 29.26
ATOM	2264 CA	ARG 1718	35.571 0.666 4 955 1 00 31.43
ATOM	2265 CB	1,10	34 632 0 210
ATOM	2266 CG		34 592 1 502
ATOM	00	1,10	34 050 3 70-
ATOM		ARG 1718	32 600 7 7 7 1.00 28.77
ATOM		ARG 1718	32 032 3 3 3 3 4 4 1.00 28.84
ATOM		ARG 1718	32 141 0 201
ATOM		ARG 1718	32 824 0 000 1.00 23.90
ATOM	_	ARG 1718	31 513 0 770
ATOM		ARG 1718	35 091 0 372
ATOM	-	ARG 1718	36 300 0 1101 1.00 33.92
•	2279 N	MET 1719	34 134 0 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
			34.134 -0.355 8.028 1.00 33.22

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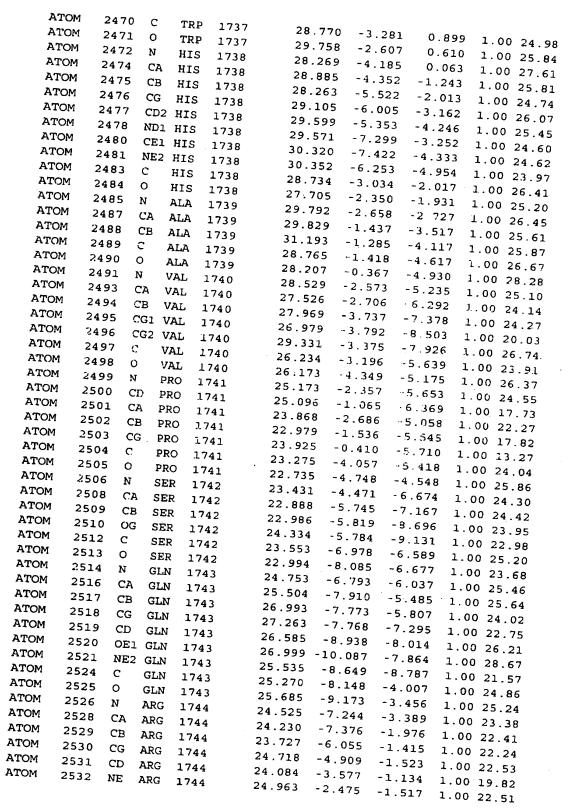
ATOM	2281	CA	MET	1719	34.428	-0.459	9.448	1.00	32.33
ATOM	2282	CB	MET	1719	33.148	-0.285	10.277	1.00	34.72
MOTA	2283	CG	MET	1719	32.454	1.066	10.076	1.00	35.04
MOTA	2284	SD	MET	1719	31.025	1.447	11.141	1.00	34.06
ATOM	2285	CE	MET	1719	29.757	0.470	10.409	1.00	33.14
ATOM	2286	С	MET	1719	35.068	-1.797	9.747	1.00	35.53
ATOM.	2287	0	MET	1719	34.896	-2.756	8.991	1.00	35.48
MOTA	2288	N	ASP	1720	35.826	-1.843	10.840	1.00	38.65
ATOM	2290	CA	ASP	1720	36.521	-3.049	11.281	1.00	39.03
MOTA	2291	CB	ASP	1720	37.659	-2.678	12.237	1.00	43.11
ATOM	2292	CG	ASP	1720	38.743	-1.846	11.569	1.00	46.69
MOTA	2293	OD1	ASP	1720	38.587	-1.536	10.364	1.00	54.08
ATOM	2294	OD2	ASP	1720	39.750	-1.503	12.239	1.00	45.93
MOTA	2295	C	ASP	1720	35.580	-4.023	11.972	1.00	38.50
MOTA	2296	0	ASP	1720	34.554	-3.617	12.528	1.00	37.73
MOTA	2297	N	LYS	1721	35.961	5.298	11.981	1.00	38.10
MOTA	2299	CA	LYS	1721	35.151	-6.339	12.600	1.00	38.12
ATOM	2300	CB	LYS	1721	35.727	-7.733	12.323	1.00	38.20
MOTA	2301	CG	LYS	1721	34.825	-8.858	12.825	1 00	38.48
ATOM	2302	CD	LYS	1721	35.375	-19.238	12.543	1.00	37.49
ATOM	2303	CE	LYS	1721	36.320	-1.0.691	13.625	1.00	39 11
MOTA	2304	NZ	LYS	1721	36.448	-12.167	13.628	1.00	40.75
ATOM	2308	С	LYS	1721	35.092	-6.142	14.091	1.00	40.24
ATOM	2309	0	LYS	1721	36.136	-6.032	14 739	1.00	42.70
MOTA	2310	N	PRO	1722	33.875	-6.082	14.658		41.23
MOTA	2311	CD	PRO	1722	32.547	-6.153	14.019	1.00	38.63
ATOM	2312	CA	PRO	1722	33.743	-5.901	16.104	1.00	41.71
MOT'A	2313	CB	PRO	1722	32.223	-5.957	16.306	1.00	38.90
ATOM	2314	CG	PRO	1722	31.679	-5.442	15.016	1.00	34.19
ATOM	2315	C	PRO	1722 .	34.418	-7.079	16.819	1.00	43.96
ATOM	2316	0	PRO	1722	34.542	-8.174	16.250	1.00	43.02
MOTA	2317	N	SER	1723	34.915	-6.860	18.028	1.00	46.76
ATOM	2319	CA	SER	1723	35.493	-7.973	18.747	1.90	50.74
MOTA	2320	CB	SER	1723	36.265	-7.500	19.980		49.47
ATOM	2321	OG	SER	1723	35.400	-7.130	21.035		53.87
ATOM	2323	С	SER	1723	34.259	-8.782	19.143		53.24
ATOM	2324	0	SER	1723	33.136	-8.259	19.130	1.00	53.97
ATOM	2325	N	ASN	1724	34.443	-10.064	19.426	1.00	56.59
ATOM	2327	CA	ASN	1724		-10.899	19.825	1.00	59.55
ATOM	2328	CB	ASN	1724		-10.386	21.162		66.12
ATOM	2329	CG	ASN	1724		-10.128	22.213		71.34
ATOM	2330		ASN	1724		-10.990	22.485		73.38
ATOM	2331	ND2		1724	33.831	-8.926	22.779		74.19
ATOM	2334	С	ASN	1724		-10.900	18.711		57.31
ATOM	2335	0	ASN	1724		-10.662	18.940		59.27
ATOM	2336	N	CYS	1725	32.723	-11.132	17.493		54.50
ATOM	2338	CA	CYS	1725	31.881	-11.203	16.300		50.89
ATOM	2339	CB	CYS	1725	31.827	-9.848	15.576		50.09
ATOM	2340	SG	CYS	1725	30.893	-9.833	14.006		44.81
MOTA	2341	С	CYS	1725		-12.235	15.439		47.28
MOTA	2342	0	CYS	1725		-12.172	15.288		48.97
ATOM	2343	N	THR	1726	31.863	-13.229	14.950	1.00	42.60

3.000		
ATOM 234		32 455
ATOM 234	6 CB THR 1726	32.3/2 -14.275 14 120 1 12
ATOM 234	7 OG1 THR 1726	31.520 -15.494 13 994 1
ATOM 234	9 CG2 THR 1726	30.290 -15.087 13 362 1 22
ATOM 235	0 C THR 1726	31.210 -16.084 15 326 1 20
ATOM 235		32.858 -13.748 12 776 1 00
ATOM 235	N ASN 1727	32.3/3 -12.704 12 357
ATOM 2354	CA ASN 1727	33./24 -14.473 12.000 3
ATOM 2355	CD 3-55	34.133 -14.044 10.742 7.00 37.02
ATOM 2356	60	35.290 -14.880 10 221 1 22
ATOM 2357	1,2/	36.580 -14.593 10.953 1.55
ATOM 2358	MD2 Post	37.188 -13.539 10.781 1 22
ATOM 2361	C 7517	37.010 -15 536
ATOM 2362	1/2/	32.958 -14.150
ATOM 2363	112/	32.883 -13 431
ATOM 2365	0.30 1/28	32.041 -15 076 39.53
ATOM 2366	CA GLU 1728	30.854 -15 310
ATOM 2367	CB GLU 1728	30.109 -16 -51
ATOM 2368	CG GLU 1728	28.973 -17.000 9.765 1.00 32.82
ATOM 2369	CD GLU 1728	28.329 -19 306 - 1.00 35.84
ATOM 2370	OE1 GLU 1728	28.409 18 633
Ti CTCODA	OE2 GLU 1.728	27.734 -18.006
T Most	C GLU 1728	29 925 1. 8.440 1.00 38.81
1000	O GLU 1728	29 521 77 9.313 1.00 33.05
	N LEU 1729	29 600 15 8.272 1.00 29 58
'i more	CA LEU 1729	28 743
7.000	CB LEU 1729	28 351 12.330 10.710 1.90 32.44
	CG LEU 1729	27 211 22.369 12.170 1.00 32.64
A MONA	CD1 LEU 1729	27 121 23.431 12.575 1.00 34.65
ATOM	CD2 LEU 1729	25 999 14.089 1.00 37.18
	C LEU 1729	20 350 11.842 1.00 27 77
	O LEU 1729	*** *** 404 10 17E 1 00
3 00014	N TYR 1730	<del>-</del> 0.36/ 4.663
ATOM 2384	A TYR 1730	10.251 1 00 34 70
	CB TYR 1730	31.378 -9.959 9.734 1.00 20 10
	CG TYR 1730	32.849 -9.940 10.154 1.00 27.22
	D1 TYR 1730	33.391 -8.723 9.649 1.00 35 55
ATOM 2388 C	E1 TYR 1730	7.449 9.879 1 00 27 37
ATOM 2389 C	D2 TYR 1730	33.725 -6.324 9.378 1 00 37 56
ATOM 2390 C	E2 TYR 1730	34.759 -8.849 8.904 1.00 34.07
ATOM 2391 C	Z TYR 1730	35.408 -7.724 8 393
ATOM 2392 O		34.882 -6.462 8.631 1.00 20
ATOM 2394 C	TYR 1730	35.473 -5.316 8.111 1.00 20.56
ATOM 2395 O		31.287 -9.962 9.200
ATOM 2396 N		31.062 -8.928 7 595 1 00
ATOM 2398 C		31.443 -11.139 7 622 13.00 29.16
ATOM 2399 CF	1731	31.366 -11.313 6 107 1 00
ATOM 2400 CG	1/21	31.611 -12.779 5 840 3 00
ATOM 2401 SD	7/27	31.315 -13.149 4 403 1 00
ATOM 2402 CE	1/31	31.801 -14.840 3 994 1 95
ATOM 2403 C	1/31	32.926 -14.502 2.606 1.00 64.38
ATOM SAS	MET 1731	29 992 10 852
ATOM See	MET 1731	29.863 -10.360
2405 N	MET 1732	28 971 _ 11 1
		28.971 -11.153 6.501 1.00 33.32
SSSD/55145		

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MOTA	2407	CA	MET	1732	27.594	-10.770	6.194	1.00 31.78
MOTA	2408	CB	MET	1732	26.634	-11.346	7.236	1.00 30.42
MOTA	2409	CG	MET	1732	25.172	-11.071	6.938	1.00 30.28
MOTA	2410	SD	MET	1732	24.071	-11.709	8.183	1.00 27.41
MOTA	2411	CE	MET	1732	23.738	-13.369	7.471	1.00 22.35
MOTA	2412	C	MET	1732	27.484	-9.243	6.158	1.00 31.10
ATOM	2413	0	MET	1732	26.794	-8.680	5.303	1.00 31.08
MOTA	2414	N	MET	1733	28.139	-8.586	7.114	1.00 31.22
ATOM	2416	CA	MET	1733	28.161	-7.128	7.189	1.00 30.93
ATOM	2417	CB	MET	1733	29.001	-6.665	8.376	1.00 31.91
ATOM	2418	CG	MET	1733	28.368	-6.906	9.710	1.00 33.63
ATOM	2419	SD	MET	1733	29.375	-6.210	11.021	1.00 34.53
ATOM	2420	CE	MET	1733	29.106	-7.395	12.280	1.00 34.12
ATOM	2421	C	MET	1733	28.830	-6.623	5.921	1.00 32.49
MOTA	2422	0	MET	1733	28.357	-5.682	5.281	1.00 33.61
MOTA	2423	N	ARG	1734	29.932	-7.269	5.551	1.00 32.11
ATOM	2425	CA	ARG	1734	30.673	-6.889	4.355	1.00 31.13
MOTA	2426	CB	ARG	1734	32.012	-7.623	4.308	1.00 28.68
ATOM	2427	CG	ARG	1734	32.953	-7.267	5.451	1. 00 27.19
ATOM	2428	CD	ARG	1734	33.159	-5.766	5.558	1.00 26.80
ATOM	2429	NE	ARG	1734	33.864	-5.243	4.393	1.00 35.67
MOTA	2431	CZ	ARG	1734	35.187	-5.305	4.223	1.00 38.03
MOTA	2432	NH1	ARG	1734	35.967	-5.861	5.148	1 00 38.07
ATOM	2435	NH2	ARG	1734	35.729	-4.850	3.094	1.00 38.87
ATOM	2438	C	ARG	1734	29.873	-7.098	3.065	1.00 29.53
MOTA	2439	O	ARG	1734	30.029	-6.334	2.121	1.00 29.11
ATOM	2440	N	ASP	1735	29.036	-8.137	3.025	1.00 29.48
ATOM	2442	CA	ASP	1735	28.193	-8.412	1.859	1.00 26.82
ATOM	2443	CB	ASP	1735	27.591	-9.811	1.933	1.00 30.25
ATOM	2444	CG	ASP	1735	28.632	-10.895	1.773	1.00 35.13
MOTA	2445		ASP	1735	29.626	-10.645	1.052	1.00 35.19
ATOM	2446		ASP	1735		-11.990	2.366	1.00 39.35
MOTA	2447	C	ASP	1.735	27.082	-7.375	1.760	100 23.88
ATOM	2448	0	ASP	1735		-6.992	0.656	1.00 24.83
ATOM	2449	N	CYS	1736	26.574	-6.929	2.913	1.00 22.13
ATOM	2451	CA	CYS	1736	25.538	-5.887	2.965	1.00 21.74
ATOM	2452	CB	CYS	1736	25.005	-5.692	4.401	1.00 20.46
ATOM	2453	SG	CYS	1736	23.978	-7.013	5.053	1.00 19.59
ATOM	2454	C	CYS	1736	26.104	-4.542	2.456	1.00 20.51
ATOM	2455	0	CYS	1736	25.377	-3.732	1.887	1.00 16.07
MOTA	2456	N	TRP	1737	27.401	-4.325	2.670	1.00 21.58
ATOM	2458	CA	TRP	1737	28.080	-3.113	2.248	1.00 20.57
ATOM	2459	CB	TRP	1737	29.107	-2.682	3.291	1.00 17.02
ATOM	2460	CG	TRP	1737	28.558	-2.415	4.654	1.00 20.35
ATOM	2461	CD2		1737	29.254	-2.564	5.897	1.00 20.42
ATOM	2462	CE2		1737	28.387	-2.122	6.923	1.00 21.18
MOTA	2463	CE3		1737	30.538	-3.027	6.243	1.00 21.60
ATOM	2464	CD1		1737	27.317	-1.914	4.970	1.00 19.86
ATOM	2465	NEI		1737	27.210	-1.732	6.328	1.00 21.03
ATOM	2467	CZ2		1737	28.760	-2.125	8.276	1.00 21.70
ATOM	2468	CZ3		1737	30.910	-3.031	7.594	1.00 21.73
ATOM	2469	CH2	TRP	1737	30.025	-2.584	8.588	1.00 23.06



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ATOM	2534	CZ	ARG	1744	24.592	-1.201	-1.663	1.00 22.92
MOTA	2535	NH1	ARG	1744	23.332	-0.814	-1.458	1.00 18.28
ATOM	2538	NH2	ARG	1744	25.491	-0.310	-2.060	1.00 22.15
MOTA	2541	C	ARG	1744	23.163	-8.458	-1.833	1.00 24.61
ATOM	2542	0	ARG	1744	22.428	-8.755	-2.786	1.00 26.94
MOTA	2543	И	PRO	1745	23.143	-9.155	-0.688	1.00 23.21
ATOM	2544	CD	PRO	1745	24.052	-9.107	0.470	1.00 22.38
MOTA	2545	CA	PRO	1745	22.129	-10.190	-0.522	1.00 22.24
MOTA	2546	CB	PRO	1745	22.623	-10.942	0.711	1.00 21.13
MOTA	2547	CG	PRO	1745	23.286	-9.864	1.504	1.00 20.24
ATOM	2548	С	PRO	1745	20.800	-9.506	-0.256	1.00 23.11
MOTA	2549	0	PRO	1745	20.743	-8.300	0.020	1.00 25.93
ATOM	2550	N	THR	1746	19.724	-10.256	-0.373	1.00 20.82
ATOM	2552	CA	THR	1746	18.420	-9.697	-0.112	1.00 20.47
MOTA	2553	CB	THR	1746	17 386	-10.342	-1.041	1.00 18.61
MOTA	2554	OG1	THR	1746	17.382	-11.755	-0.822	1.00 21.86
MOTA	2556	CG2	THR	1746	17.746	-10.078	-2.487	1.00 21.13
ATOM	2557	C	THR	1746	18.060	-9.970	1.344	1.00 20.84
ATOM	2558	0	THR	1746	18.787	-10.674	2.055	1.00 22.08
ATOM	2559	N	PHE	1747	16.953	-9.406	1.810	1.00 21.58
MOTA	2561	CA	PHE	1747	16.536	-9.675	3.178	1.00 21.15
ATOM	2562	CB	PHE	1747	15.442	-8.710	3.613	1.00 20 34
MOTA	2563	CG	PHE	1747	15.961	-7.350	3.982	1.00 23.18
ATOM	2564	CD1	PHE	1747	16.729	-7 170	5.130	1.00 22.26
ATOM	2565	CD2	PHE	1747	15.668	-6.240	3.196	1.00 23.41
MOTA	2566	CE1	PHE	.1747	17.186	-5.909	5.484	1.00 17.31
ATOM	2567	CE2	PHE	1747	15.124	-4.967	3.548	1.00 17.93
MOTA	2568	CZ	PHE	1747	16.883	-4.809	4.696	1.00 19.06
MOTA	2569	С	PHE	1747	16.062	-11.124	3.217	1.00 21.61
ATOM	2570	O	PHE	1747	16.248	-11.823	4.212	1.00 22.19
ATOM	2571	N	LYS	1748	15.490	-11.588	2.111	1.00 22.00
ATOM	2573	CA	LYS	1748	15.048	-12.973	2.009	1.00 24.34
ATOM	2574	CB	LYS	1748		-13.227	0.621	1.00 23.61
ATOM	2575	CG	LYS	1748		-14.663	0.416	1.00 27.45
MOTA	2576	CD	LYS	1748		-14.932	-0.998	1.00 28.97
ATOM	2577	CE	LYS	1748		-16.394	-1.163	1.00 35.95
ATOM	2578	NZ	LYS	1748		-16.795	-0.153	1.00 41.69
MOTA	2582	Ç	LYS	1748		-13.907	2.264	1.00 27.58
MOTA	2583	0	LYS	1748		-14.863	3.034	1.00 29.73
ATOM	2584	N	GLN	1749		-13.604	1.640	1.00 25.88
ATOM	2586	CA	GLN	1749		-14.394	1.804	1.00 23.72
ATOM	2587	CB	GLN	1749		-13.925	0.837	1.00 27.00
ATOM	2588	CG	GLN	1749		-13.954	-0.628	1.00 32.28
ATOM	2589	CD	GLN	1749		-13.331	-1.477	1.00 36.35
ATOM	2590		GLN	1749		-12.528	-2.368	1.00 37.63
ATOM	2591	NE2		1749		-13.702	-1.194	1.00 38.60
ATOM	2594	C	GLN	1749		-14.266	3.212	1.00 23.44
ATOM	2595	0	GLN	1749		-15.260	3.826	1.00 23.52
ATOM	2596	N	LEU	1750		-13.035	3.703	1.00 21.73
ATOM	2598	CA	LEU	1750		-12.796	5.054	1.00 20.90
ATOM	2599	CB	LEU	1750		-11.308	5.359	1.00 18.60
ATOM	2600	CG	LEU	1750	20.654	-10.439	4.485	1.00 16.53

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ימ	TOM	
	TOM 2601 CD1 LEU 1750	20.190 -8.979 4 579 1 22
	TOM 2602 CD2 LEU 1750	22 100 13.28
	TOM 2603 C LEU 1750	18 003 10.612 4.939 1.00 14.74
	TOM 2604 O LEU 1750	10.534 6.108 1.00 21.25
	IOM 2605 N VAI. 1751	7 084 1 00 00
	OM 2607 CA VAL 1751	-13,50/ 5 917 1 00 0-
	OM 2608 CB VAL 1751	14.209 6 845 1 00 ca
	OM 2609 CG1 VAL 1751	14.0/2 6.432 1.00
AT	OM 2610 CG2 VAL 1751	14.3/0 / 220 1 00 00
AT	OM 2611 C VAI. 1751	12.048 6 684 1 00
ATO	OM 2612 O VAL 1751	17.127 -15.774 6 925 3 00 ==
ATO	OM 2613 N GLII 1752	369 8 007 1 00
ATC	OM 2615 CA GLU 1752	1/.418 -16.381 5 778 1 00 25
ATC	OM 2616 CB GLU 1752	17.773 -17.789 5 755 1 00 5
ATO	OM 2617 CG GLU 1752	17.765 -18.317 4.321 1.00 ==
ATO	M 2610 1732	16.399 -18.218 3.651 3.00
ATO	M 3610 OHO 1/52	16.394 -18.742 2.216 1.00 44.76
ATO	M 2620 CD2 ***	15.397 -18.495 1 497 + 22 ==
ATO	M 3631 -	17.377 -19.419
ATO	M 2022 2	19 140 17 00:
ATO	M 2522 M 250 1752	19 330 10 000
ATO	M 2625 (IR	20 069 -17 006
ATOM	1 2626 CR ASP 1753	21 411 12 224
ATOM	1 2627 CC 100	22 341 16 144
ATOM	1 2628 OD1 305	22 498 -16 350
ATOM	1 3630 1753	22 222
ATOM.	3630 T	22 908 -15 405
ATOM	3631 c ASP 1753	21 379 36 305
ATOM	3632 ASP 1753	21 971 22 272
ATOM	2624	20 652 -15 070
ATOM	3635 m	20 568 -15 722
ATOM	2626	19 881 14 301
ATOM	2636 CG LEU 1754	20 810 33 33-
ATOM	2637 CD1 LEU 1754 2638 CD2 LEU 1754	20 045 11 000
ATOM	2020 1734	21,932 -12,162
ATOM	2639 C LEU 1754	19.860 -16.070 1.00 25.69
ATOM	2640 O LEU 1754	20 270 -17 220
ATOM	2641 N ASP 1755	18 824 17 42
ATOM	2643 CA ASP 1755	18 109 10 510
ATOM	2644 CB ASP 1755	16 944 19 030
ATOM	2645 CG ASP 1755	16 100 20 00-
ATOM	2646 OD1 ASP 1755	15 771 10 01
ATOM	2647 OD2 ASP 1755	15 817 20 00-
ATOM	2648 C ASP 1755	19 040 10 700
	2649 O ASP 1755	10.000 19.703 10.952 1.00 32.29
ATOM	2650 N ARG 1756	19 926 10 000 11.979 1.00 31.66
ATOM	<sup>2652</sup> CA ARG 1756	9,989 1 00 20 -
ATOM	2653 CB ARG 1756	21 500 21.015 10.059 1.00 32.73
ATOM	2654 CG ARG 1756	22 722 - 8.704 1.00 34.47
ATOM	2655 CD ARG 1756	8.645 1.00 25 -
ATOM	2656 NE ARG 1756	23.299 -22.274 7 237 1 00 10
ATOM	2658 CZ ARG 1756	23.791 -20.999 6 702 1 20
ATOM	2659 NH1 ARG 1756	24.890 -20.380 7 122 1 00 7
		25.630 -20.914 8.091 1.00 55.88
_		-100 33.08

MOTA	2662	NH2	ARG	1756	25.237	-19.214	6.593	1.00 52.53
MOTA	2665	С	ARG	1756	21.889	-20.761	11.186	1.00 33.76
ATOM	2666	0	ARG	1756	22.131	-21.619	12.049	1.00 34.53
ATOM	2667	N	ILE	1757	22.432	-19.553	11.204	1.00 33.49
MOTA	2669	CA	ILE	1757	23.405	-19.176	12.205	1.00 32.71
MOTA	2670	CB	ILE	1757	23.980	-17.764	11.919	1.00 31.86
ATOM	2671	CG2	ILE	1757	25.111	-17.454	12.869	1.00 31.71
ATOM	2672	CG1	ILE	1757	24.520	-17.704	10.488	1.00 31.41
ATOM	2673	CD1	ILE	1757	25.075	-16,366	10.096	1.00 27.68
MOTA	2674	С	ILE	1757	22.807	-19.236	13.604	1.00, 34.20
MOTA	2675	0	ILE	1757	23.399	-19.833	14.495	1.00 35.83
ATOM	2676	N	VAL	1758	21.620	-18.667	13.792	1.00 35.40
ATOM	2678	CA	VAL	1758	20.981	-18.653	15.108	1.00 37.49
ATOM	2679	CB	VAL	1758	19.501	-18.160	15.061	1.00 34.42
ATOM	2680	CG1	VAL	1758	18.899	-18.199	16.456	1.00 37.37
ATOM	2681	CG2	VAL	1758	19.403	-16.742	14.519	1.00 30.02
MOTA	2682	С	VAL	1758	21.010	-20.050	15.715	1.00 41.64
MOTA	2683	0	VAL	1758	21.533	-20.246	16.817	1.00 43.69
MOTA	2684	N	ALA	1759	20.492	-21.015	14 961	1.00 44.52
MOTA	2686	CA	ALA	1759	20.434	-22.415	15.387	1.00 45.20
MOTA	2687	CB	ALA	1759	19.833	-23.268	14.277	1.00 43.44
MOTA	2688	C	ALA	1759	21.791	-22.968	15.795	1.00 45.91
MOTA	2689	0	ALA	1759	21.890	-23.780	16.710	1.00 47.41
ATOM	2690	N	LEU	1760	22.833	-22.511	15.120	1.00 47.70
MOTA	2692	CA	LEU	1760	24.190	-22.960	15.399	1.00 50.91
MOTA	2693	CB	LEU	1760	25.015	-22.912	14.109	1.00 52.93
ATOM.	2694	CG	LEU	1760	24.448	-23.723	12.947	1.00 57.55
MOTA	2695	CD1	LEU	1760 .	25.189	-23.390	11.660	1.00 60.76
ATOM	2696	CD2	LEU	1760	24.539	-25.208	13.273	1.00 58.66
ATOM	2697	C	LEU	1760	24.882	-22.111	16.472	1.00 52.07
ATOM	2698	O	LEU	1760	25.967	-22.459	16.953	1.00 51.95
ATOM	2699	N	THR	1761	24.267	-21.000	16.850	1.00 52.05
MOTA	2701	CA	THR	1761	24.868	-20.131	17.836	1.00 53.28
ATOM	2702	CB	THR	1761	24.362	-18.693	17.673	1.00 54.58
MOTA	2703	OG1	THR	1761	24.633	-18.259	16.339	1.00 53.68
ATOM	2705	CG2	THR	1761	25.090	-17.762	18.621	1.00 55.45
MOTA	2706	С	THR	1761	24.715	-20.619	19.272	1.00 53.31
ATOM	2707	0	THR	1761	23.629	-20.986	19.713	1.00 53.89
ATOM	2708	N	SER	1762	25.832	-20.617	19.993	1.00 53.51
ATOM	2710	CA	SER	1762	25.876	-21.045	21.383	1.00 53.15
ATOM	2711	CB	SER	1762	27.340	-21.131	21.830	1.00 57.27
MOTA	2712	OG	SER	1762	27.492	-21.872	23.028	1.00 61.22
MOTA	2714	С	SER	1762	25.110	-20.048	22.257	1.00 49.15
MOTA	2715	0	SER	1762	25.229	-18.831	22.071	1.00 46.61
ATOM	3466	N	ALA	461	79.636	26.047	14.493	1.00 61.05
ATOM	3468	CA	ALA	461	79.609	24.852	13.654	1.00 58.10
ATOM	3469	CB	ALA	461	78.335	24.024	13.935	1.00 60.39
ATOM	3470	C	ALA	461	79.694	25.239	12.179	1.00 54.65
ATOM	3471	0	ALA	461	79.653	24.382	11.297	1.00 54.05
ATOM	3472	N	ALA	462	79.867	26.537	11.935	1.00 51.68
MOTA	3474	CA	ALA	462	79.972	27.085	10.584	1.00 48.47
ATOM	3475	CB	ALA	462	80.099	28.619	10.633	1.00 46.99
								- · · - <del>-</del>

ATO		476	C .	ALA	462	81.:	מ כנו		_			
ATC	_	477	0	ALA	462	80.9		6.489		766	1.00	44.86
ATC		178	N	ΓΥR	463	82.3		6.097			1.00	43.40
ATO	-	180	CA :	'YR	463	83.4		6.447			1.00	42.23
ATO		181		YR	463	84.6		5.913			1.00	39.04
ATO		82		'YR	463	84.3		6.921		20	1.00	39.01
ATO		83	CD1 1	YR	463	84.0		8.126			1.00	41.95
ATO		84	CE1 T	YR	463	83.7		9.373		08 ]	1.00	42.40
ATO			CD2 T		463	84.3		0.466			00	42.02
OTA		86	CE2 T	_	463	83.9		8.009				40.70
ATO		87 (	CZ T		463	83.7		9.099				37.09
ATON			T HC		463	83.40		0.320	7.13		.00	39.19
ATOM		90 (	T		163	84.0		406	6.36		.00	40.66
ATOM		91 (	) T:		163	84.62		.554	10.05		.00	37.78
ATOM		92 N	J GI		64	83.74		.863	9.23		.00	38.35
ATOM	-	34 (	A GI		64	84.21		143	11.28			37.67
ATOM		)5 C	B GI		64	85.70		.841	11.74		.00	38.57
ATOM	_	6 C	G GL		64	86.09		.890	12.02		00 4	11.44
ATOM		_	D GL	U 4	64	87.58		.870	13.10			7.87
ATOM			E1 GL	U 4	64	87.99		. 135	13.16		00 5	3.44
ATOM	349		E2 GL	U 4	64 .	88.34		. 983	13.99			6.72
ATOM	350	0 C	$\operatorname{GL}$	U 4	64	83.50		. 513	12.39		00 5	4.85
ATOM	350	_	GL	U 4	64	83.29		393	13.00		00 3	8.15
ATOM	350		LE	J 4	65	83.12		187	13.905		00 3	9.59
ATOM	3504		A LE	J 46	55	82.45		.124 608	13.05			7.13
ATOM	3509		LE	J 46	55	81.502		456	14.236		00 3	7.93
ATOM	3506				55	80.455			13.894		00 3	3.43
MOTA	3507		1 LEU	J 46	55	79.415			12.787		00 3	
ATOM ATOM	. 3508				5	79.797			12.944			1.85
ATOM	3509	_	LEU		5	83.540			12.855		00 29	9.05
ATOM	3510		LEU		5	84.703			15.166 14.763		00 41	.02
ATOM	3511		PRO	_		83.198			16.441		0.0 40	
ATOM	3512			46	6	81.974	20		17.115		0 43	
ATOM	3513	CA		46		84.170	19.3		17.415		0 45	
ATOM	3514	CB	PRO	46		83.433	19.5		18.743	1.0	0 44	.72
ATOM	3515 3516	CG	PRO	46		82.486	20.6		18.496	1.0	0 46	.18
ATOM	3517	C	PRO	460		84.447	17.9		7.101	1.0	0 48	. 84
ATOM	3518	O N	PRO	466		83.616	17.2		6.509	1.0	0 <b>4</b> 4 0 <b>4</b> 3	. 52
ATOM	3520	CA	GLU	467		85.610	17.4		7.492	1.0		
ATOM	3521		GLU	467		85.932	16.0		7.218		0 47	
ATOM	3522	CB CG	GLU	467		87.354	15.9		6.659	1.00	0 56.	. 03
ATOM	3523	CD	GLU	467		87.615	14.5		6.000	1 00	62.	. 11
ATOM	3524		GLU GLU	467		88.927	14.4		5.242	1 00	66.	.27
ATOM	3525	OET	GLU	467		89.688	15.4		5.243	1.00	, 66. 1 60	39
ATOM	3526	C C		467		89.182	13.4		4.643	1 00	66.	00
ATOM	3527	0	GLU	467		85.749	15.13		8.435		49.	
ATOM	3528	N	GLU	467		85.767	15.60		9.578	1.00	49.	62
ATOM	3530	CA	ASP	468		85.516	13.85		3.166	1.00	<b>⊒</b> ⊅.	02
ATOM	3531		ASP	468		85.352	12.84		9.198	1.00		
ATOM	3532	CB CG	ASP	468		83.880	12.67		587	1.00		
ATOM	3533	OD1	ASP	468		83.678	11.74		779	1.00	45.	. o
		ODI	MOL	468		82.544	11.70		.309	1.00		
											72.(	J-4

ATOM	3534	OD2	ASP	468	84.629	11.033	21.188	1.00 38.14
MOTA	3535	С	ASP	468	85.877	11.556	18.580	1.00 45.54
MOTA	3536	0	ASP	468	85.141	10.815	17.928	1.00 45.94
ATOM	3537	N	PRO	469	87.181	11.308	18.732	1.00 45.89
ATOM	3538	CD	PRO	469	88.111	12.189	19.464	1.00 45.11
ATOM	3539	CA	PRO	469	87.885	10.130	18.215	1.00 45.91
ATOM	3540	CB	PRO	469	89.208	10.187	18.968	1.00 45.90
ATOM	3541	CG	PRO	469	89.456	11.662	19.042	1.00 45.73
ATOM	3542	C	PRO	469	87.170	8.806	18.473	1.00 45.48
ATOM	3543	0	PRO	469	87.188	7.905	17.629	1.00 46.83
ATOM	3544	N	ARG	470	86.495	8.717	19.613	1.00 42.12
MOTA	3546	CA	ARG	470	85.786	7.506	19.999	1.00 41.21
MOTA	3547	CB	ARG	470	85.083	7.704	21.331	1.00 43.14
MOTA	3548	CG	ARG	470	85.885	8.424	22.375	1.00 45.68
ATOM	3549	CD	ARG	470	85.014	8.705	23.564	1.00 45.98
ATOM	3550	NE	ARG	470	83.802	9.417	23.184	1.00 47.28
ATOM	3552	CZ	ARG	470	82.921	9.877	24.057	1.00 50.54
ATOM	3553	NH1	ARG	470	83.127	9.687	25.354	1.00 47.56
ATOM	3556	NH2	ARG	470	81.843	10.527	23 637	1.00 54.59
ATOM	3559	С	ARG	470	84.736	7.058	19.004	1.00 40.57
ATOM	3560	0	ARG	470	84.411	5.877	18.941	1.00 43.13
ATOM	3561	N	TRP	471	84.182	8.014	18.268	1.00 38.07
ATOM	3563	C:A	TRP	471	83.124	7.736	17.314	1.00 35.09
MOTA	3564	CB	TRP	471	81.890	8.515	17.739	1.00 33.42
ATOM	3565	CG	TRP	471	81.259	7.958	18.952	1.00 31.71
ATOM	3566	CD2	TRP	471	80.512	б.740	19.026	1.00 34.81
ATOM	3567	CE2	TRP	471	80.061	6.610	20.355	1.00 33.17
ATOM	3568	CE3	TRP	471	80.174	5.744	18.092	1.00 37.60
ATOM	3569	CD1	TRP	471	81.246	8.503	20.199	1.00 25.70
ATOM	3570	NEl	TRP	471	80.525	7.697	21.051	1.00 28.79
ATOM	3572	CZ2	TRP	471	79.289	5.522	20.776	1.00 35.80
MOTA	3573	CZ3	TRP	471	79.409	4.660	18.509	1.00 35.52
MOTA	3574	CH2	TRP	471	78.973	4.560	19.839	1.00 34.51
ATOM	3575	С	TRP	471	83.432	8.065	15.872	1.00 35.77
ATOM	3576	0	TRP	471	82.690	7.670	14.968	1.00 37.45
ATOM	3577	N	GLU	472	84.533	8.770	15.651	1.00 34.76
MOTA	3579	CA	GLU	472	84.895	9.184	14.308	1.00 34.51
ATOM	3580	CB	GLU	472	86.065	10.174	14.365	1.00 32.30
MOTA	3581	CG	GLU	472	86.221	11.038	13.103	1.00 36.57
MOTA	3582	CD	GLU	472	85.082	12.035	12.872	1.00 36.34
ATOM	3583	OE1		472	84.515	12.558	13.857	1.00 36.01
ATOM	3584	OE2	GLU	472	84.777	12.318	11.694	1.00 31.95
ATOM	3585	С	GLU	472	85.219	8.034	13.364	1.00 33.90
ATOM	3586	0	GLU	472	85.896	7.082	13.745	1.00 33.77
ATOM	3587	N	LEU	473	84.667	8.094	12.158	1.00 33.58
ATOM	3589	CA	LEU	473	84.944	7.095	11.146	1.00 34.82
MOTA	3590	CB	LEU	473	83.714	6.234	10.847	1.00 32.59
MOTA	3591	CG	LEU	473	84.020	5.091	9.867	1.00 33.78
MOTA	3592	CD1	LEU	473	84.786	4.000	10.578	1.00 32.94
MOTA	3593	CD2	LEU	473	82.759	4.518	9.273	1.00 35.34
MOTA	3594	С	LEU	473	85.380	7.828	9.883	1.00 37.95
ATOM	3595	0	LEU	473	84.720	8.781	9.457	1.00 39.55

	MOTA	3596		PRO	474						
	TOM	3597	CD	PRO	474	00.	522	7.423	9.299	1 00	30.00
	TOM	3598	CA	PRO	474	٠,.	455	6.453	9.899	1.00	38.99
	TOM	3599	CB	PRO	474	87.	094	8.004	8.080	1.00	38.76
	TOM	3600	CG	PRO		88.	382	7.201	7.906	7.00	39.37
	TOM	3601	C	PRO	474	88.	767	6.883	9.310	1.00	40.18
	rom :	3602	0	PRO	474	86.	165	7.794	6.890	1.00	37.76
	rom :	3603	N	ARG	474	85.8		6.653	6.532	1.00	10.94
	гом з	8605	~-	ARG	475	85.7		8.886	6.245	1.00	13.98
ΑT	OM 3	606		ARG	475	84.8	50	8.840	5.101	1.00 4	0.66
	'ОМ 3	607		ARG	475	84.7	76 1	0.216	4.448	1.00 4	0.66
AT	'ОМ 3	608	`	ARG	475	84.3	54 1	1.300	5.415	1.00 3	7.94
AT	ОМ з	609		ARG	475	84.3	40 12	2.697	4.800	1.00 3	6.12
AT	_	611		ARG	475	83.9	32 13	3.677		1.00 3	5.92
ATO		612		ARG	475	82.6	71 13	3.878	_	1.00 3	0.14
ATO		515	NH2 A		475	81.68	38 13	.197	_	1.00 2	3.45
ATO	OM 36	518	_	RG	475	82.41	0 14	.666	_	1.00 28	3.41
ATC		19		RG	475	85.14	1 7	. 766		1.00 27	1.85
ATO	M 36			rG SP	475	84.22		_	_	1.00 41	.44
ATO			~-		476	86.41			3.470	.00 41	.40
ATO	M 36			SP SP	476	86.83			3.830 j	00 44	.99
ATO	M 36		_		476	88.34	4 6	_	2.849 1	.00 50	.62
ATO!	M 36:		ODI AS		476	89.10	5 5.		2.644 1	.00 54	.47
ATO	4 36:		DD2 AS		476	89.569	9 4.		3.819 <sub>1</sub> 3.722 <sub>1</sub>	.00 60	.03
ATOM	1 362	27		_	476	89.216		A A A		.00 65	.09
ATOM	1 362	-		_	476	86.436	5.	_	-	.00 62.	62
ATOM	362			_	476	86.678	4.			.00 51.	16
ATOM	363		A AR	_ `	177	95.900	4.			.00 53.	06
ATOM	363		B AR	~	177	85.443				00 49.	58
ATOM	363	-		_	77 .	86.040				00 47.	34
ATOM	363				77	87.481	2.9			00 48.	85
ATOM	363				77 77	88.169	3.0	\ <b>7</b> 0 -		00 52.	11
ATOM	363				77 77	87.515	2.3		665 1.	00 53.6	53
ATOM	3638	NF	II ARG		77 77	87.932	2.3			00 54.8	<b>3</b> 6
MOTA	3641		2 ARG			89.000	3.0			00 57.1	. 5
ATOM	3644		ARG		77	87.269	1.6			00 55.9	· <b>8</b>
ATOM	3645	0	ARG			83.915	3.5	_		00 58.3	1
MOTA	3646	N	LEU			83.339	2.7			0 44.7	0
MOTA	3648	CA	LEU	47		83.274	4.36			0 44.6	3
ATOM	3649	CB	LEU	47		81.832	4.44	10 4	_	0 41.9	5 -
ATOM	3650	CG	LEU	47	_	81.374	5.60			0 38.50 0 33.1	3
ATOM	3651	CD:	LEU	47		79.872	5.73	5.1		0 33.17	<i>,</i>
ATOM	3652	CD2	LEU	478		79.393	4.59	2 6.0	_	0 29.07	,
ATOM	3653	С	LEU	478		79.590	7.05	9 5.8	-	0 28.25 0 30.79	i
ATOM	3654	0	LEU	478		81.432	4.71	0 2.6		30.79	
ATOM	3655	N	VAL	479		81.938	5.64	7 2.0		38.93	
ATOM	3657	CA	VAL	479		80.562	3.88			41.75	
ATOM	3658	CB	VAL			80.113	4.086	5 0.7		37.96	
ATOM	3659		VAL	479		80.468	2.882			37.87	
ATOM	3660	CG2	VAL	479		80.001	3.145		-	36.47	
ATOM	3661	C .	VAL	479 479		81.972	2.651			34.43	
ATOM	3662	0	VAL			78.609	4.299	0.77		34.33	
				479		77.846	3.366	1.01		38.10	
SSD/551.									- 1.00	40.13	
17711/551	4E 0.										

MOTA	3663	N	LEU	480	78.184	5.537	0.552	1.00 38	3.05
ATOM	3665	CA	LEU	480	76.766	5.879	0.606	1.00 35	. 90
ATOM	3666	СВ	LEU	480	76.568	7.393	0.475	1.00 33	. 98
ATOM	3667	CG	LEU	480	77.276	8.257	1.536	1.00 32	. 84
ATOM	3668	CD1	LEU	480	77.003	9.749	1.273	1.00 29	.68
ATOM	3669	CD2	LEU	480	76.828	7.861	2.943	1.00 26	.03
ATOM	3670	C	LEU	480	76.015	5.146	-0.476	1.00 34	.99
ATOM	3671	0	LEU	480	76.573	4.864	-1.526	1.00 36	.12
ATOM	3672	N	GLY	481	74.753	4.836	-0.223	1.00 35	.21
ATOM	3674	CA.	GLY	481	73.965	4.120	-1.204	1.00 34	.79
ATOM	3675	C	GLY	481	72.544	4.608	-1.332	1.00 36	.31
ATOM	3676	0	GLY	481	72.237	5.775	-1.046	1.00 38	.30
MOTA	3677	N	LYS	482	71.665	3.705	-1.761	1.00 35	.59
ATOM	3679	CA	LYS	482	70.257	4.007	-1.959	1.00 35	. 24
MOTA	3680	CB	LYS	482	69.488	2.698	-2.207	1.00 35	.69
MOTA	3681	С	LYS	482	69.585	4.763	-0.823	1.00 36	.31
MOTA	3682	0	LYS	482	69.752	4.421	0.352	1.00 34	.90
ATOM	3683	N	PRO	483	68.787	5.786	-1.157	1.00 38	.08
MOTA	3684	CD	PRO	483	68.432	6.320	-2.483	1.00 39	
MOTA	3685	CA	PRO	483	68.097	6.566	-0.135	1.00 41	.08
A'TOM	3686	CB	PRO	483	67.300	7.560	-0.987	1.00 39	
ATOM	3687	CG	PRO	483	68.268	7.819	-2.157	1.00 37	.87
ATOM	3688	C	PRO	483	67.130	5.652	0.606	1.00 42	. 11.
MOTA	3689	0	PRO	483	66.306	4.994	-0.025	1.00 43	01
A.TOM	3690	N	LEU	484	67.199	5.624	1.937	1.00 41	. 06
MOTA	3692	CA	LEU	484	66.293	4.823	2.751	1.00 38	. 47
ATOM	3693	CB	LEU	484	67.040	4.307	3.990	1.00 32	. 45
MOTA	3694	CG	LEU	484	67.968	3.098	3.809	1.00 27	.68
ATOM	3695	CD1	LEU	484	68.569	2.710	5.147	1.00 20	.29
ATOM	3696	CD2	LEU	484	67.181	1.964	3.225	1.00 23	.20
MOTA	3697	С	LEU	484	65.084	5.637	3.180	1.00 42	.18
MOTA	3698	O	LEU	484	65.227	6.699	3.814	1.00 44	.50
MOTA	3699	N	GLY	485	63.893	5.170	2.817	1.00 45	.68
MOTA	3701	CA	GLY	485	62.692	5.863	3.220	1.00 49	
ATOM	3702	C	GLY	485	62.216	7.008	2.337	1.00 53	.01
MOTA	3703	O	GLY	485	62.438	7.005	1.117	1.00 50	.26
MOTA	3704	N	GLU	486	61.592	8.020	2.949	1.00 56	. 24
ATOM	3706	CA	GLU	486	61.064	9.183	2.257	1.00 58	
MOTA	3707	CB	GLU	486	59.666	8.845	1.682	1.00 55	.60
ATOM	3708	C	GLU	486	60.995	10.477	3.088	1.00 59	
ATOM	3709	0	GLU	486	60.019	11.226	3.000	1.00 61	
ATOM	3710	N	GLY	487	62.027	10.747	3.879	1.00 59	
ATOM	3712	CA	GLY	487	62.066	11.964	4.652	1.00 59	. 75
ATOM	3713	С	GLY	487	61.337	11.959	5.974	1.00 61	. 44
ATOM	3714	0	GLY	487	61.231	12.979	6.627	1.00 61	. 96
ATOM	3715	N	ALA	488	60.820	10.800	6.377	1.00 59	
ATOM	3717	CA	ALA	488	60.134	10.709	7.657	1.00 57	
ATOM	3718	CB	ALA	488	59.489	9.337	7.825	1.00 58	
ATOM	3719	C	ALA	488	61.137	10.970	8.754	1.00 56	
MOTA	3720	0 +	ALA	488	60.810	11.446	9.834	1.00 57	
ATOM	3721	N	PHE	489	62.389	10.630	8.480	1.00 54	
ATOM	3723	CA	PHE	489	63.462	10.830	9.466	1.00 54	. 56

> man.	
ATOM 3724 CB PHE 489	<b>a</b>
ATOM 3725 CG DUE	9,500 9 770 1
ATOM 3726 CD1 pro-	63.222 8.454 10 352 1 22
ATOM 3727 403	62.505 7.585 9.516 7.50 45.21
ATOM 3720 489	63.017
ATOM 3729 CF2	61.625 5 653 1.00 40.99
ATOM 2720 - 489	62.138 7.433
ATOM 3737 7 PHE 489	61 423 4 12.257 1.00 35.02
ATOM 3733	64 456 13 25 11.407 1.00 34.73
ATOM 3735 PHE 489	65 372 12 55 8.974 1.00 56.31
	2.2/6 9.692 1 00 50 5-
CA GLY 40A	7,735 1 00 55 55
3/36 C GIV	7.143 1 00 55 60
ATOM 3737 () CLV	55.899 12.778 5.993 1.00 54.75
ATOM 3738 N GIN	05.35/ 11.854 5 366
ATOM 3740 CA CLAY	67.073 13.304 5 634
ATOM 3741 CB CIN	67.829 12 550
ATOM 3742 CG GTV	68.760 13 500
ATOM 3743 - 491	69,422 12 010 53.48
MON (19)	70.046 13.506 2.629 1.00 57.19
Amon OEI GLN 491	70.113 14.003 1.548 1.00 62.09
ATOM 371	70 452 12 1 1.701 1.00 70.26
GLN 491	68 632 11 - 0.441 1.00 62.78
OLN 401	59.660 1. 5.165 1.00 49.89
N VAL 493	5.805 1 00 40 75
7752 TA VAL 492	4.984 1 00 47 55
3753 CB VAL 492	9.093 5.456 1 00 46 33
3754 CG1 TAT	8.320 6.412 1.00 45.61
ATOM 3755 CG2 VAY	7.045 6 933
ATOM 3756 C VAL 402	9.211 7.605
ATOM 3757 0	69.004 8.200 4 353
ATOM 3758 N 1757	68.181 8.044 3.340 3.65
ATOM 3760 CA VAL	70.210 7.654 4.309 1.50 45.17
ATOM 3761 CB VAL 493	70.599 6 780 1.00 43.75
7004	71.608 7.471
Amou CGL VAL 493	71.159 9 900 2.148 1.00 46.20
ATOM 375 CG2 VAL 493	73.045 7.439 1.00 46.16
ATOM ADD VAL 493	71.205 5 402 2.706 1.00 42.06
ATOM 3754	71 701 5 3.624 1.00 44.09
5700 N LEU 494	71 102 4.745 1.00 43.73
ATOM STORE CA LEU 494	71 602 - 2.809 1.00 43.38
CB LEU 494	70 990 3.142 1.00 43 29
3770 CG LEU 494	2.030 2.366 1.00 43.30
3771 CD1 LEU 494	2.431 1 00 30
ATOM 3772 CD2 FRIT 40	/1.809 0.201 3.850
ATOM 3773 C T.ETT 46.	70.600 -0.337 1 750
ATOM 3774 O LED 404	73.139 3.280 2 725
A10M 3775 N ATA 405	73.435 3.929 1 720 1 720
ATOM 3777 CA ALA 495	74.044 2.698 3.490 1.00 43.83
ATOM 3778 CB N.D.	75.456 2.785 3.193 1.00 40.80
ATOM 3779 C ALA 495	76.059 4.032 3.103 1.00 43.80
ATOM 3780 0 378	76, 171 1 546 3.021 1.00 43.76
ATOM 3702	75.668 0.030 3.682 1.00 46.68
ATOM STOR GLU 496	77.330 1.350 4.551 1.00 48.52
ATOM 370	79 112 3.104 1.00 49 13
ATOM 3784 CB GLU 496	78 524
	78.524 -0.732 2.318 1.00 53.83

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ATOM	3785	CG	GLU	496	77.350	-1.224	1.496	1.00 61.33
ATOM	3786	CD	GLU	496	77.623	-2.561	0.862	1.00 64.74
MOTA	3787		GLU	496	76.704	-3.411	0.883	1.00 70.08
MOTA	3788		GLU	496	78.751	-2.760	0.356	1.00 64.12
MOTA	3789	С	GLU	496	79.333	0.601	4.230	1.00 48.46
MOTA	3790	0	GLU	496	80.192	1.236	3.631	1.00 48.79
MOTA	3791	N	ALA	497	79.373	0.375	5.530	1.00 49.25
MOTA	3793	CA	ALA	497	80.503	0.810	6.334	1.00 49.99
MOTA	3794	CB	ALA	497	80.048	1.156	7.732	1.00 48.16
ATOM	3795	C	ALA	497	81.544	-0.301	6.373	1.00 51.53
ATOM	3796	0	ALA	497	81.191	-1.473	6.409	1.00 52.41
ATOM	3797	N	ILE	498	82.821	0.061	6.335	1.00 52.35
ATOM	3799	CA	ILE	498	83.892	-0.928	6.369	1.00 52.03
ATOM	3800	CB	ILE	498	84.843	-0.797	5.145	1.00 52.83
ATOM	3801	CG2	ILE	498	85.990	-1.795	5.253	1.00 51.43
MOTA	3802	CG1	ILE	498	84.077	-1.006	3.830	1.00 53.85
ATOM	3803	CD1	ILE	498	83.411	0.254	3.271	1.00 55.62
ATOM	3804	C	ILE	498	84.702	-0.802	7.654	1.00 52.74
ATOM	3805	0	ILE	498	85.133	0.293	8.026	1.00 52.14
ATOM	3806	N	GLY	499	84.835	-1.926	8.354	1.00 52.58
ATOM	3808	CA	GLY	499	85.600	-1.974	9.592	1.00 53.03
MOTA	3809	C	GLY	499	85.165	-1.113	10.771	1.00 53.67
ATOM	3810	O.	GLY	499	86.012	-0.544	11.463	1.00 53.99
ATOM	3811	N	LEU	500	83.862	-1.045	11.034	1.00 53.60
MOTA	3813	CA	LEU	500	83.337	-0.245	12.141	1.00 51.00
MOTA	3814	CB	LEU	500	81.841	-0.499	12.317	1.00 49 38
MOTA.	3815	CG	LEU	500	80.901	-0.024	11.212	1.00 47.62
MOTA	3816	CD1	LEU	500	79.483	-0.454	11.543	1.00 47.25
MOTA	3817	CD2	LEU	500	80.992	1.486	11.081	1.00 47.38
MOTA	3818	C	LEU	500	84.060	-0.573	13.433	1.00 51.05
ATOM	3819	0	LEU	500	84.396	-1.734	13.670	1.00 53.76
ATOM	3820	N	PRO	505	87.588	-5.968	10.545	1.00 81.81
ATOM	3821	CD	PRO	505	88.588	-6.677	11.357	1.00 81.96
ATOM	3822	CA	PRO	505	88.105	-4.664	10.109	1.00 80.56
ATOM	3823	CB	PRO	505	89.501	-4.622	10.735	1.00 80.75
ATOM	3824	CG	PRO	505	89.868	-6.070	10.860	1.00 82.32
ATOM	3825	С	PRO	505	88.139	-4.477	8.588	1.00 78.53
MOTA	3826	0	PRO	505	88.462	-3.400	8.085	1.00 77.85
MOTA	3827	N	ASN	506	87.792	-5.532	7.865	1.00 77.09
ATOM	3829	CA	ASN	506	87.747	-5.484	6.411	1.00 75.57
ATOM	3830	CB	ASN	506	88.799	-6.415	5.806	1.00 75.80
ATOM	3831	С	ASN	506	86.347	-5.929	6.008	1.00 74.33
ATOM	3832	0	ASN	506	86.044	-6.117	4.826	1.00 73.76
ATOM	3833	N	ARG	507	85.496	-6.092	7.018	1.00 71.72
ATOM	3835	CA	ARG	507	84.120	-6.509	6.820	1.00 69.28
ATOM	3836	CB	ARG	507	83.619	-7.257	8.054	1.00 70.64
ATOM	3837	C	ARG	507	83.258	-5.284	6.605	1.00 65.87
MOTA	3838	0	ARG	507	83.445	-4.262	7.274	1.00 65.40
ATOM	3839	N	VAL	508	82.363	-5.358	5.628	1.00 62.01
ATOM	3841	CA	VAL	508	81.464	-4.248	5.381	1.00 58.41
MOTA	3842	CB	VAL	508	81.043	-4.136	3.915	1.00 57.18
ATOM	3843	CG1		508	82.251	-3.893	3.046	1.00 61.04
						5.555	3.040	00 01.04

	TOM 3844		AL 508	9.0	210 -	_	
	TOM 3845	C V				383 3.46	56 1.00 60.74
	COM 3846			80.			16 1.00 56.61
	OM 3847	N TH		79.			9 1.00 55.82
	OM 3849	CA TH	- 4 5	79.		501 6.66	
AT	OM 3850	CB TH		78.:		510 7.50	
AT		OG1 TH		78.7		144 8.93	
AT		CG2 TH		79.9		727 9.35	
AT	OM 3854	C TH		77.€		65 9.90	
ATO	OM 3855	O THI		77.3	81 -2.6		/.5/
ATO	DM 3856			77.6	75 -1.5		
ATO	DM 3858			76.2	38 -3.2		10.09
ATC				75.2	02 -2.3		
ATO		CB LYS		74.0			
ATO		CG LYS		73.2			
ATO		CD LYS		73.82		•	
ATO		CE LYS		73.13			- 50.33
ATO		NZ LYS	510	73.31			,,,,,
ATO	,	C LYS	510	74.73			
ATO	-0.70	O LYS	510	74.48		_	
ATO		N VAL	511	74.67	_		1.00 38.59
ATOM	- · · -	CA VAL	511	74.26		_	1.00 36.28
ATOM	. 5072	CB VAL	511	75.48	_		1.00 31.41
ATOM		CG1 VAL	511	76.31			1.00 32.80
		CG2 VAL	511	76.35	_		1.00 29.97
ATOM		C VAL	511	73.40			1.00 30.20
ATOM	5070	O VAL	511	73.305			1.00 28.40
ATOM		V ALA	512	72.756			1.00 27 45
ATOM	•	ALA	512	71.953			1.00 27.30
MOTA	3880 (	B ALA	512	70.557			1.00 26.66
ATOM	3881	ALA	512				1.00 24.24
ATOM	3882 (	ALA	512	72.670			1.00 28.52
ATOM	3883 N	VAL	513	73.140	_		1.00 26.66
ATOM	3885 C	A VAL	513	72.768			1.00 29.18
ATOM	3886 C	B VAL	513	73.442		7.569	1.00 29.65
ATOM	3887 C	G1 VAL	513	74.631	7.482	6.601	1.00 28.93
ATOM		G2 VAL	513	75.384	8.722	7.015	1.00 25.51
ATOM	3889 C	VAL	513	75.570	6.292	6.550	1.00 29.45
ATOM	3890 O	VAL	513	72.509	8.407	7.476	1.00 30.45
ATOM	3891 N	LYS	514	71.900	8.646	6.431	1.00 30.15
ATOM	3893 C		514	72.402	9.143	8.578	1.00 33.29
ATOM	3894 CE		514	71.575	10.357	8.654	1.00 33.28
ATOM	3895 CG		514	71.017	10.537		1.00 38.67
ATOM	3896 CD	_		70.074	9.456		1.00 45.73
ATOM	3897 CE		514	69.462	9.860		1.00 53.93
ATOM	3898 NZ		514	68.450	8.840		00 63.59
ATOM	3902 C	_	514	67.206	8.823		.00 71.90
MOTA	3903 O	LYS	514	72.451	11.568		00 20 45
ATOM	3904 N		514	73.584	11.673		.00 29.45
ATOM	2.2		515	71.918	12.495		.00 25.64
ATOM	-		515	72.668	13.690		.00 29.42
ATOM	•		515	73.464	13.391		.00 30.46
ATOM			515	72.557	13.070		.00 29.63
	3909 SD	MET	515		12.475	4.665 1 3.218 1	.00 32.48
						3.218 ]	.00 33.06

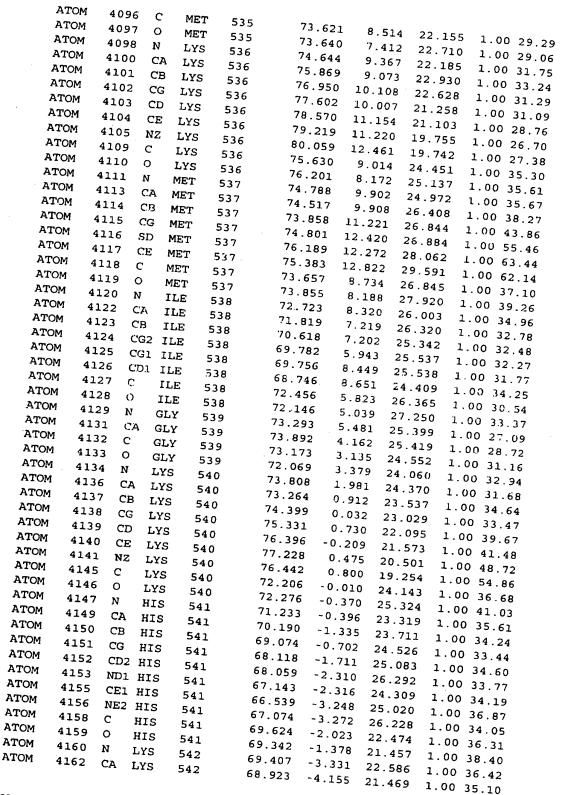
ATOM	3910	CE	MET	515	73.734	10.809	3.715	1.00 30.26
ATOM	3911	C	MET	515	71.700	14.839	6.848	1.00 30.75
MOTA	3912	0	MET	515	70.478	14.654	6.867	1.00 33.07
ATOM	3913	N	LEU	516	72.238	16.027	6.608	1.00 30.32
ATOM	3915	CA	LEU	516	71.414	17.194	6.304	1.00 30.21
MOTA	3916	CB	LEU	516	72.112	18.487	6.748	1.00 26.54
ATOM	3917	CG	LEU	516	72.452	18.668	8.227	1.00 23.97
ATOM	3918	CD1	LEU	516	73.345	19.858	8.412	1.00 24.27
MOTA	3919	CD2	LEU	516	71.198	18.850	9.023	1.00 21.46
ATOM	3920	С	LEU	516	71.197	17.265	4.800	1.00 33.44
MOTA	3921	0	LEU	516	72.016	16.784	4.015	1.00 34.50
ATOM	3922	N	LYS	517	70.082	17.863	4.400	1.00 36.36
MOTA	3924	CA	LYS	517	69.783	18.048	2.993	1.00 34.58
ATOM	3925	CB	LYS	517	68.281	18.255	2.784	1.00 38.96
ATOM	3926	CG	LYS	517	67.409	17.155	3.380	1.00 44.34
MOTA	3927	CD	LYS	517	66.128	16.920	2.572	1.00 52.11
MOTA	3928	CE	LYS	517	65.138	18.083	2.637	1.00 58.29
ATOM	3929	NZ	LYS	517	63.915	17.833	1.786	1.00 60.90
ATOM	3933	С	LYS	517	70.567	19.304	2.597	1.00 33.51
ATOM	3934	0	LYS	517	71.024	20.064	3.460	1.00 30.34
ATOM	3935	N	SER	518	70.701	19.539	1.296	1.00 34.39
ATOM	3937	CA	SER	518	71.444	20.693	0.788	1.00 35.84
ATOM	3938	СВ	SER	518	71.537	20.618	-0.731	1.00 33.66
ATOM	3939	OG	SER	518	70.282	20.258	-1.266	1.00 38.73
ATOM	3941	C	SER	518	70.879	22.045	1.198	1.00 36.91
ATOM	3942	ပ်	SER	518	71.591	23.050	1.205	1.00 37.32
MOTA	3943	N	ASP	519	69.598	22.069	1.538	1.00 37.88
MOTA	3945	CA	ASP	519	68.945	23.313	1.936	1.00 38.63
MOTA	3946	CB	ASP	519	67.517	23.364	1.375	1 00 42.23
ATOM	3947	CG	ASP	519	66.669	22.151	1.775	1.00 48.87
ATOM	3948	001	ASP	519	67.070	21.380	2.681	1.00 49.21
ATOM	3949		ASP	519	65.582	21.972	1.181	1.00 54.93
ATOM	3950	C	ASP	519	68.916	23.537	3.443	1.00 38.06
ATOM	3951	0	ASP	519	68.246	24.451	3.916	1.00 39.38
ATOM	3952	N	ALA	520	69.622	22.692	4.191	1.00 36.24
ATOM	3954	CA	ALA	520	69.631	22.795	5.648	1.00 34.69
ATOM	3955	CB	ALA	520	70.359	21.613	6.259	1.00 35.68
ATOM	3956	C	ALA	520	70.213	24.087	6.173	1.00 33.54
ATOM.	3957	ō	ALA	520	71.039	24.718	5.522	1.00 34.83
ATOM	3958	N	THR	521	69.815	24.452	7.384	1.00 34.45
ATOM	3960	CA	THR	521	70.315	25.668	8.001	1.00 34.43
ATOM	3961	CB	THR	521	69.148	26.592	8.493	1.00 30.31
ATOM	3962	OG1		521	68.529	26.031	9.659	1.00 33.14
ATOM	3964		THR	521	68.081	26.750	7.409	1.00 41.61
ATOM	3965	C	THR	521	71.228	25.303		
ATOM	3966	0	THR	521	71.376		9.170 9.510	1.00 36.35
ATOM	3967	Ŋ	GLU	521 522	71.868	24.125	9.510 9.756	1.00 32.23
ATOM	3969	CA	GLU	522 522		26.310		1.00 39.33
ATOM	3970	CB			72.747	26.092	10.890	1.00 44.59
ATOM			GLU	522	73.364	27.424	11.335	1.00 51.80
	3971	CG	GLU	522	74.463	27.311	12.418	1.00 64.10
ATOM	3972	CD	GLU	522	75.811	26.815	11.886	1.00 69.12
ATOM	3973	OE1	GLU	522	76.784	27.605	11.869	1.00 69.26

Δ.	ATOM 39			
		74 OE2		75.900 25.629 11.500
	mov.	75 C	GLU 522	73 053 11.302 1.00 73.62
	ma		GLU 522	72 402 23.447 12.042 1.00 44 53
		77 N	LYS 523	24.61/ 12.786 1 00 44 05
	TOM 39	70	LYS 523	70.679 25.814 12.167 1 00 42 00
A:	TOM 39			09.826 25.264 13 216 1 00
A	TOM 391	0.1		68.519 26.053 13 329 1 00
A	70M 398			67.583 25 502 1.00 45.99
	OM 398		LYS 523	66.296 25 027 1.00 48.74
	OM 398		LYS 523	65,405, 34,303
AT			YS 523	64 309 22 505
AT	_	· - L	YS 523	69 562 25.586 14.247 1.00 65.17
			YS 523	69 501 23.753 [2.935 1.00 39.03
AT		ONA	SP 524	22.9/3 13.850 1 00 40 65
ATO	-	2 C'A A	SP 524	69.331 23 457 11.672 1 00 34 03
AT(	OM 399		SP 524	69.122 22.068 11 294 1 20
ATO	DM 3994			08.876 21.942 9 790
ATO	OM 3999	OD1 AS		67.482 22.352 4 380 1 34.84
ATC	DM 3996			66.552 22 202
ATO		71		67.307 22.025
ATO	,			70.383 27 304 - 0.240 1.00 38.19
ATO				70.301 20.104
ATO				71 554 12.139 1.00 37.40
ATO			Ծ 525	72 700 11.404 1.00 32.39
		CB LE	U 525	1.186 11.729 1 00 31 50
ATO	-	CG LE		21.998 11.278 1.00 29 05
ATO		CD1 LE		75.363 21.375 11.680 1.00 29 20
ATOM	4005	CD2 LET		75.521 19.990 11 065 1 22 25
ATOM	4005	C LET		76.519 12.283 11.795 1.00 27.27
ATOM			25	72.848 30.941 13 221 1
ATOM	4008			73.104 10.006
ATOM				72.563 21.000 13.075 1.00 33.58
ATOM		CA SER	- = 0	72.544 21 224
ATOM	_	CB SER		72.046 22.25
ATOM	·	OG SER		71.923 22.100 == 1.00 32.03
ATOM		C SER	526	71 (40 23.139 17.417 1.00 37.02
	4015	O SER	526	71 004 15.980 1.00 29.72
ATOM	4016	N ASP	527	20.162 16.998 1.00 27.54
ATOM	4018	CA ASP	527	70.525 20.588 15.291 1 00 20 07
ATOM	4019	CB ASP	527	69.581 19.556 15.664 1 00
ATOM	4020	CG ASP		68.289 19.720 14 BEE 1
ATOM	4021	OD1 ASP	527	67.497 20.977 15 225 1 20 2
ATOM		OD2 ASP	527	67.750 21.597 16 303 1.00 30.05
ATOM			527	66.591 21.335 14 436 1 24.32
ATOM			527	70 175 19 164 1.00 34.69
ATOM	4	O ASP	527	70.115 17 208 1.00 30.65
ATOM	400-	N LEU	528	70.769 17.000 -0.312 1.00 30.12
		CA LEU	528	71 250 14.265 1.00 30.50
ATOM		CB LEU	528	71 050 10.669 13.946 1.00 29.54
ATOM	4029 (	CG LEU	528	
ATOM	4030	CD1 LEU	528	72.409 15.320 11 842 3
ATOM	4031	D2 LEU	528	71.466 14.142 12.259 1.00 21 51
ATOM	4032 C			/2.644 15.437 10.450 1.00
ATOM	4033 0		528	72.494 16.342 14 922 1 22
ATOM	4034 N		528	72 641 75 700 30.51
ATOM			529	73 281 17 25
	±030 (	A ILE	529	74 367 17 13
				74.367 17.138 16.253 1.00 28.41
CCCD !				

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PCT/US97/14885

MOTA	4037	CB	ILE	529	75.266	18.349	16.406	1.00 24.75	
MOTA	4038	CG2	ILE	529	<b>76.35</b> 5	18.064	17.432	1.00 25.51	
MOTA	4039	CG1	ILE	529	75.901	18.710	15.084	1.00 17.82	
ATOM	4040	CD1	ILE	529	76.912	19.806	15.251	1.00 18.14	
MOTA	4041	С	ILE	529	73.821	16.813	17.641	1.00 30.17	
ATOM	4042	0	ILE	529	74.286	15.873	18.285	1.00 30.11	
ATOM	4043	N	SER	530	72.836	17.574	18.101	1.00 30.29	
ATOM	4045	CA	SER	530	72.271	17.310	19.418	1.00 33.14	
ATOM	4046	CB	SER	530	71.158	18.293	19.735	1.00 36.09	
MOTA	4047	OG	SER	530	70.224	18.323	18.670	1.00 49.01	
ATOM	4049	C.	SER	530	71.740	15.881	19.479	1.00 33.80	
MOTA	4050	Ú	SER	530	71.896	15.190	20.492	1.00 37.06	
ATOM	4051	N	GLU	531	71.156	15.413	18.378	1.00 30.13	
MOTA	4053	CA	GLU	531	70.629	14.065	18.351	1.00 29.18	
ATOM	4054	CB	GLU	531	69.822	13.801	17.087	1.00 32.42	
ATOM	4055	CG	GLU	531	69.253	12.394	17.058	1.00 33.35	
MOTA	4056	CD	GLU	531	68:354	12.131	15.883	1.00 34.76	
MOTA	4057	OE1	GLU	531	67.481	11.249	16.002	1.00 40.42	
MOTA	4058	OE2	GLU	531	68.516	121793	14.847	1.00 35.88	
ATOM	4059	C	GLU	531	71.734	13.025	18.488	1.00 28.27	
ATOM	4060	0	GLU	531	71.569	12.032	19.192	1.00 26.75	
ATOM	4061	N	MET	532	72.842	13.235	17.786	1.00 27.80	
ATOM	4063	CA	MET	532	73.976	12.320	17.835	1.00 27.82	
ATOM	4064	CB	MET	532	75.080	12.813	16.890	1.00 29.43	
MOTA	4065	CG	MET	532 .	76.461	1.2.225	17.138	1.00 24.34	
ATOM	4066	SD	MET	532	77.641	12.702	15.840	1.00 27.83	1
MOTA	4067	CE	MET	532	77.791.	14.452	16.193	1.00 21.90	
ATOM	4068	С	MET	532	74.499	12.272	19.260	1.00 29.53	
ATOM	4069	0	MET	532	74.742	11.197	19.809	1.00 30.14	
ATOM	4070	N	GLU	533	74.610	13.445	19.871	1.00 30.25	
ATOM	4072	CA	GLU	533	75.109	13.570	21.233	1.00 31.95	
ATOM	4073	CB	GLU	533	75.300	15.039	21.594	1.00 32.55	
ATOM	4074	CG	GLU	533	76.391	15.724	20.765	1.00 35.71	
ATOM	4075	CD	GLU	533	77.766	15.087	20.951	1.00 36.71	
MOTA	4076	OE1	GLU	533	78.297	15.136	22.084	1.00 40.19	
MOTA	4077	OE2	GLU	533	78.322	14.555	19.969	1.00 33.99	
ATOM	4078	С	GLU	533	74.185	12.886	22.225	1.00 33.06	
ATOM	4079	0	GLU	533	74.642	12.197	23.147	1.00 33.49	
ATOM	4080	N	MET	534	72.883	13.052	22.025	1.00 33.12	
ATOM	4082	CA	MET	534	71.913	12.432	22.900	1.00 32.48	
ATOM	4083	CB	MET	534	70.484	12.859	22.533	1.00 30.60	
ATOM	4084	CG	MET	534	69.591	12.915	23.791	0.50 28.70	PRT1
ATOM	4085	SD	MET	534	67.787	12.849	23.608	0.50 27.55	PRT1
ATOM	4086	CE	MET	534	67.409	14.560	23.291	0.50 26.84	PRT1
ATOM	4087	С	MET	534	72.102	10.908	22.785	1.00 31.10	
ATOM	4088	0	MET	534	72.258	10.224	23.791	1.00 32.80	
MOTA	4089	N	MET	535	72.194	10.394	21.563	1.00 30.50	
MOTA	4091	CA	MET	535	72.399	8.961	21.368	1.00 29.25	
ATOM	4092	CB	MET	535	72.577	8.623	19.884	1.00 28.10	
ATOM	4093	CG	MET	535	71.337	8.876	19.042	1.00 27.48	
MOTA	4094	SD	MET	535	71.377	7.980	17.502	1.00 26.94	
ATOM	4095	CE	MET	535	71.346	9.275	16.310	1.00 33.72	



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MOTA	4163	CB	LYS	542	68.680	-5.602	21.915	1.00	34.24
MOTA	4164	C	LYS	542	67.674	-3.646	20.802	1.00	32.40
ATOM	4165	0	LYS	542	67.507	-3.822	19.612	1.00	32.37
ATOM	4166	N	ASN	543	66.785	-3.046	21.580	1.00	32.12
ATOM	4168	CA	ASN	543	65.541	-2.561	21.015	1.00	33.01
ATOM	4169	CB	ASN	543	64.361	-3.081	21.842	1.00	
ATOM	4170	CG	ASN	543	64.365	-4.597	21.979	1.00	32.20
ATOM	4171	OD1	ASN	543	64.633	-5.128	23.050	1.00	32.23
ATOM	4172		ASN	543	64.077	-5.292	20.904	1.00	30.50
MOTA	4175	Ċ	ASN	543	65.424	-1.050	20.719	1.00	32.21
ATOM	4176	0	ASN	543	64.326	-0.481	20.765		31.13
ATOM	4177	N	ILE	544	66.556	-0.419	20.397	1.00	30.52
ATOM	4179	CA	ILE	544	66.611	1.002	20.028	1.00	29.01
ATOM	4180	CB	ILE	544	67.040	1.962	21.208	1.00	25.83
ATOM	4181	CG2	ILE	544	66.244	1.682	22.467	1.00	
ATOM	4182	CG1	ILE	544	68.532	1.848	21.522	1.00	
ATOM	4183	CD1	ILE	544	69.008	2.839	22.581	1.00	
ATOM	4184	C	ILE	544	67.617	1.118	18.870	1.00	23.49
ATOM	4185	0	ILE	544	68.410	0.194	18.€33	1.00	27.26
MOTA	4186	N	ILE	545	67.504	2.184	18.078	1.00	28.74
ATOM	4188	CA	ILE	545	68.453	2.396	16.992		27.06
ATOM	4189	CB	ILE	545	67.913	3.350	15.921		23.64
ATOM	4190	CG2	ILE	545	69.027	3.727	14.955		23.96
ATOM	4191	CG1		545	66.754	2.692	15.167	1.00	23.13
ATOM	4192		ILE	545	67.152	1.481	14.339	1.00	
ATOM	4193	C	ILE	545	69.720	2.968	17.633		26.93
ATOM	4194	Ö	ILE	545	69.719	4.075	18.160		28.63
ATOM	4195	N	ASN	546	70.800	2.200	17.560		28.53
ATOM	4197	CA	ASN	546	72.075	2.567	18.161		29.39
ATOM	4198	СВ	ASN	546	72.752	1.308	18.718		29.14
ATOM	4199	CG	ASN	546	71.908	0.613	19.772		30.21
ATOM	4200		ASN	546	71.804	1.088	20.899		30.74
ATOM	4201		ASN	546	71.290	-0.505	19.406		30.79
ATOM	4204	С	ASN	546	73.034	3.303	17.238		30.78
ATOM	4205	0	ASN	546	73.011	3.126	16.015		33.04
ATOM	4206	N	LEU	547	73.866	4.151	17.837		31.07
ATOM	4208	CA	LEU	547	74.880	4.904	17.101		31.37
MOTA	4209	СВ	LEU	547	75.284	6.165	17.875		27.32
ATOM	4210	CG	LEU	547	76.413	7.032	17.297		24.17
ATOM	4211	CD1		547	75.953	7.768	16.069		18.06
ATOM	4212	CD2		547	76.864	8.014	18.348		22.50
ATOM	4213	С	LEU	547	76.107	3.999	16.861	1.00	
MOTA	4214	0	LEU	547	76.610	3.343	17.789	1.00	
MOTA	4215	N	LEU	548	76.543	3.919	15.607		32.72
ATOM	4217	CA	LEU	548	77.694	3.104	15.259	1.00	
ATOM	4218	CB	LEU	548	77.388	2.244	14.029	1.00	
ATOM	4219	CG	LEU	548	76.148	1.341	14.158	1.00	
ATOM	4220	CD1		548	76.034	0.513	12.906	1.00	
ATOM	4221	CD2		548	76.196	0.436	15.394	1.00	
ATOM	4222	C	LEU	548	78.941	3.965	15.030		33.69
ATOM	4223	0	LEU	548	80.063	3.488	15.167	1.00	
ATOM	4224	N	GLY	549	78.746	5.229	14.675	1.00	
	7	••	J	J 7 J	70.740	3.443	14.0/3	1.00	24.10

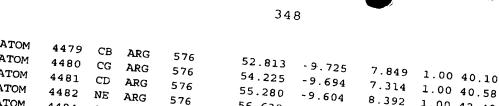
ATOM 4226 CD CD	
ATOM CA GLY 54	9 79.871 6.116 14.45
ATOM 1335 GLY 54	9 70 14.454 1 00 31
ATOM GLY 54	9 73.425 7.429 13.839 1 00 31.30
4229 N ALA 55	7.686 12 700
4231 CA ALA EF	00.388 8.268 13 474
4232 CB ATA -	9.540 13 050
ATOM 4233 C ALA FE	79.537 10.526 13.800
4234 O ATA -	81.257 10 140 1.00 27.87
ATOM 4235 N CVG	82,422 9 943 1.00 27.66
ATOM 4237 CD 351	80.944 10.830 12.4/4 1.00 25.24
ATOM 4238 CP CH 551	81.924 11 540 10.984 1.00 27.61
ATOM 4239 CO 551	81.754 11 337 10.1/0 1.00 25.02
ATOM 4240 - 015 351	82 155 0 0 0 0 1 00 22 41
ATOM 4241 (1 515 551	81 582 3 6.18/ 1.00 27 24
ATOM 4242 551	10.447 1 00 0
ATOM 4244 THR 552	9,958 1 00 00
ATOM ADDITIONAL THR 552	- 41.303 7 00 00
ATOM 4245 CB THR 552	15.046 11.664 1 00 25.22
4246 OG1 THR 550	15.215 13.202 1 00 00
4248 CG2 THR 553	05.479 15.031 13.664 1 00 25
4249 C THR 553	01.23/ 14.171 13 006
ATOM 4250 C THR 552	83.134 16.014 17 000
4251 N Ct 1	82.894 17.216 11 005
4253 CA GLN 553	84.264 15.473 10.562
4254 CB GLN 553	85.355 16.288 10.153 4.00 30.26
ATOM 4255 CG CT 11	86.669 15.768 10.763
ATOM 4256 CD CT	86.653 15 crc 300 29.54
ATOM 4257 OF 1 01-1	86.534 17.007
4258 NDC 31 3	87.440 17 831 1.00 26.86
ATOM 4261 C CV	85.421 17 220 1.00 30.85
ATOM 4262 0 CIN 553	85.475 16 216 13.676 1.00 23.89
ATOM 4263 N 353	85.221 15 313 - 6.634 1.00 28.30
ATOM 4265 CD 200	85.860 17.480
ATOM 4266 - 354	86 070 17 77
ATOM ASP 554	87 370 17 00 0.695 1.00 27 85
ATTOM	88 534 17 - 6.257 1 00 33 44
ATOM 1275 ODI ASP 554	7.060 1 00 27
ATOM 1000 554	0.763 1 00 40 -
ATOM 4275 ASP 554	0.000 1 00 1
42/1 O ASP 554	5.715 1 00 00
42/2 N GLY EEC	03.193 16.518 4.826 1 00 21
42/4 CA GLV	03.824 17.981 5.842 1.00 38.55
44/5 C GLY 566	02.720 17.694 4.949 1.00 07
42/6 O GLY EEF	5.734 1 00 00
ATOM 4277 N PPO 555	81.423 17.795 6 941 1.00 23.07
A10M 4278 CD DDG	80.338 17.185 5.036
ATOM 4279 Ch PRO	80.280 16.750 3 670 22.81
ATOM 4280 CB DDG	/9.039 17.032 5 773
ATOM 4281 CG PRO	78.154 16.499 4 610 1.00 23.99
ATOM 4282 C PRO 556	79.144 15.801 3.602 1.00 22.41
ATOM 4283 O DDO	79.080 16.066 3.698 1.00 24.36
ATOM 4284 N 1711	79.854 15 111 6.911 1.00 26.98
ATOM 4286 CD 557	78.237 16.335 5.934 1.00 28.57
ATOM 4207 - 557	78.168 15 455 7.896 1.00 29.25
1110M 4287 CB LEU 557	77 550 36 30 9.070 1.00 30 83
	77.550 16.225 10.251 1.00 33.20
SSSD/55145. v01	

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ATOM	4288	CG	LEU	557	77.109	15.416	11.475	1.00 30.01
MOTA	4289	CD1	LEU	557	78.304	14.793	12.174	1.00 29.05
ATOM	4290	CD2	LEU	557	76.365	16.341	12.407	1.00 29.20
ATOM	4291	С	LEU	557	77.324	14.238	8.780	1.00 30.33
MOTA	4292	0	LEU	557	76.175	14.343	8.330	1.00 27.66
MOTA	4293	N	TYR	558	77.913	13.071	9.002	1.00 30.68
MOTA	4295	CA	TYR	558	77.214	11.823	8.812	1.00 29.26
ATOM	4296	CB	TYR	558	77.978	10.933	7.840	1.00 30.99
ATOM	4297	CG	TYR	558	78.066	11.481	6.430	1.00 35.01
ATOM	4298	CD1	TYR	558	79.108	11.109	5.592	1.00 36.17
ATOM	4299	CE1	TYR	558	79.198	11.600	4.296	1.00 41.40
ATOM	4300	CD2	TYR	558	77.109	12.368	5.941	1.00 36.44
ATOM	4301	CE2	TYR	558 .	77.188	12.871	4.648	1.00 40.96
MOTA	4302	CZ	TYR	558	78.237	12.484	3.825	1.00 43.59
MOTA	4303	ОН	TYR	558	78.298	12.965	2.525	1.00 42.91
MOTA	4305	C	TYR	558	77.081	11.125	10.164	1.00 28.18
ATOM	4306	0	TYR	558	78.077	10.855	10.835	1.00 28.06
MOTA	4307	N	VAL	559	75.842	10.879	10.574	1.00 26.72
ATOM	4309	CA	VAL	559	75.548	10.175	31.821	1.00 26.72
MOTA	4310	CB	VAL	559	74.326	10.813	12.552	1.00 28.03
ATOM	4311		VAL	559	73.915	9.992	13.771	1.00 29.85
ATOM	4312		VAL	559	74.655	12.236	12.982	1.00 29.37
ATOM	4313	C	VAL	559	75.238	8.723	11.443	1.00 25.58
MOTA	4314	0	VAL	559	74.131	8.402	10.988	1.00 25.73
ATOM	4315	N	ILE	560	76.214	7.851	11.642	1.00 24.35
ATOM	4317	CA	ILE	560 560	76.061	6.448	11.281	1.00 26.64
ATOM	4318	CB	ILE	560	77.441	5.781	11.002	1.00 26.53
MOTA MOTA	4319 4320	CG2 CG1	ILE	560 560	77.252	4.359	10.465	1.00 27.80
ATOM	4321	CDI	ILE	560	78.254 79.671	6.620 6.112	10.004 9.763	
ATOM	4321	C	ILE	560	75.312	5.633	12.339	1.00 17.05 1.00 27.95
ATOM	4323	0	ILE	560	75.777	5.493	13.479	1.00 27.95
ATOM	4324	N	VAL	561	74.163	5 084	11.951	1.00 23.10
ATOM	4326	CA	VAL	561	73.352	4.265	12.847	1.00 27.43
ATOM	4327	CB	VAL	561	72.048	5.000	13.251	1.00 25.08
ATOM	4328		VAL	561	72.367	6.302	13.936	1.00 19.97
ATOM	4329		VAL	561	71.186	5.250	12.033	1.00 25.55
ATOM	4330	C	VAL	561	73.031	2.896	12.202	1.00 30.21
ATOM	4331	0	VAL	561	73.404	2.623	11.045	1.00 32.04
ATOM	4332	N	GLU	562	72.306	2.062	12.944	1.00 28.88
MOTA	4334	CA	GLU	562	71.940	0.714	12.509	1.00 27.69
ATOM	4335	CB	GLU	562	71.448	-0.081	13.712	1.00 26.79
ATOM	4336	CG	GLU	562	72.387	0.001	14.873	1.00 28.13
ATOM	4337	CD	GLU	562	72.012	-0.916	16.003	1.00 31.86
MOTA	4338		GLU	562	72.772	-1.876	16.255	1.00 33.17
ATOM	4339	OE2	GLU	562	70.974	-0.654	16.639	1.00 35.50
ATOM	4340	С	GLU	562	70.898	0.636	11.405	1.00 27.34
ATOM	4341	0	GLU	562	69.990	1.453	11.358	1.00 29.72
ATOM	4342	N	TYR	563	71.002	-0.392	10.568	1.00 28.07
ATOM	4344	CA	TYR	563	70.080	-0.626	9.455	1.00 32.50
ATOM	4345	СВ	TYR	563	70.848	-1.236	8.269	1.00 28.32
ATOM	4346	CG	TYR	563	70.042	-1.427	7.007	1.00 26.56

ATOM 4347 CD1 THE	
ATTOM CDI TYR 56	69.338 -0.378 6 442
ATOM 1340 CEI TYR 56	3 68 620 5.448 1.00 30 40
ATOM 4355 CD2 TYR 56	3 70 011 5.258 1.00 32 82
ATOM 4355	3 60 61 2.032 6.350 1 00 20 65
ATOM 10-1 CZ TYR 56	3 50 - 2.021 5.151 1.00 20
ATOM 4352 OH TYR 56	3 -1.755 4.619 1 00 22 -
Amore 4354 C TYR 56	3.460 1 00 40
1701 4355 O TYR 56	00.930 -1.564 9.878 1 00 26 25
4356 N ALA 564	09.151 -2.569 10.562 1 00 36
ATOM 4358 CA ALA 564	9.454 1 00 20
ATOM 13 CB ALA 564	9.750 1 00 35
ATOM ATA 564	
ATOM 135	03.919 -2.360 8.394 1.00 43
ATOM 1361 N SER 565	7.977 1 00 47.61
ATOM 4364 CA SER 565	7.745 1 00 45
ATOM 4365 CB SER 565	3.806 6.421 1.00 45
4366 OG SER 565	55.134 6.070 7.00 45
4368 C SER 565	7.1/5 1 00 33
4369 O SER BCF	6.164 1 00 40
ATOM 4272 LYS 566	53.823 5.025 1 00 45
ATOM LYS 566	/.19/ 1 00 30 -
ATOM 4374 TO LYS 566	6.392 1 00 00
ATOM AS 566	7.783 3 00 35
ATOM 4376 566	62 163 0 7.308 1.00 38 21
ATOM 4377 566	62 734 2 8.208 1.00 38 79
ATOM 4393 TO 195 566	62.600 30 76
ATOM 1205 LYS 566	61 400 3 598 1.00 42 40
ATOM 4302 U LYS 566	60 265 1.00 37 29
ATOM 4205 - 567	62 166 1.415 1.00 39 49
ATOM 4396 CA GLY 567	61 407 - 1.00 34 37
ATOM 4387 0 STEE	60.810 -0.423 7.428 1.00 32.82
ATOM 4388 N NO.	61.251 -1.012
ATOM 4390 CA AGY	59.722 0.304 5.778 1.00 29.23
ATOM 4391 CP 30.8	58.999 0 500 8.754 1.00 29.92
ATOM 4392 CG ACN 568	58.414 1 203 31.05
ATOM 4393 ODI 202	57.201 2.157 9.007 1.00 31.23
ATOM 4394 ND2 703	56.095 1.685 9.305
4397 C ACM	57.394 2.877 7.000 1.00 37.22
ATOM 4398 O 2017	57.950 -0.405
A1019 4399 N TETT	57.535 -1.205 9 324
A10M 4401 CA 7 DY	57.517 -0.548 37 400
ATOM 4402 CR TETT	56.540 -1.511 31 070
ATOM 4403 CG IEU	56.456 -1.408 73 500
4404 CD1 LEU 560	55.509 -2.363 14 210 36.13
4405 CD2 THE	56.010 -3.804 14.034
ATOM 4406 C LEU 560	55.425 -1.971 15 664
ATOM 4407 O TEX	55.141 -1.420 11 202 -
4408 N ARG 570	54.518 -2.447 11 141
ATOM 4410 CA ARC FOR	54.636 -0.213 11 162
ATOM 4411 CB ARG 570	53.299 -0.063 10 503
ATOM 4412 CG ARG 570	52.979 1.403 10 321
	51.558 1 620 39.48
SSSD/55145, v01	1.638 9.887 1.00 41.93

MOTA	4413	CD	ARG	570	51.459	2.966	9.182	1.00 49.89
ATOM	4414	NE	ARG	570	52.329	2.991	8.009	1.00 55.25
ATOM	4416	CZ	ARG	570	53.121	4.008	7.693	1.00 57.90
ATOM	4417	NH1	ARG	570	53.145	5.093	8.455	1.00 56.93
ATOM	4420	NH2	ARG	570	53.921	3.920	6.637	1.00 57.58
ATOM	4423	С	ARG	570	53.219	-0.835	9.278	1.00 39.84
MOTA	4424	0	ARG	570	52.309	-1.644	9.060	1.00 42.48
ATOM	4425	N	GLU	571	54.208	-0.597	8.425	1.00 38.22
ATOM	4427	CA	GLU	571	54.292	-1.251	7.135	1.00 38.84
MOTA	4428	СВ	GLU	571	55.284	-0.492	6.266	1.00 40.72
MOTA	4429	CG	GLU	571	54.818	0.941	5.999	1.00 49.17
ATOM	4430	CD	GLU	571	55.845	1.798	5.284	1.00 58.95
ATOM	4431	OE1	GLU	571	57.047	1.434	5.278	1.00 67.07
ATOM	4432	OE2	GLU	571	55.455	2.854	4.736	1.00 61.02
ATOM	4433	C	GLU	571	54.617	-2.744	7.240	1.00 37.79
ATOM	4434	C	GLU	571	54.075	-3.558	6.488	1.00 37.63
ATOM	4435	N	TYR	572	55.462	-3.104	8.204	1.00 36.89
MOTA	4437	CA	TYR	572	55.841	-4.498	8.437	1.00 36.81
ATOM	4438	CB	TYR	572	56.822	-4.584	9.612	1.00 33.24
ATOM	4439	CG	TYR	572	57.191	-5.987	10.080	1.00 33.42
MOTA	4440	CD1	TYR	572	58.209	-6.714	9.450	1.00 31.93
ATOM	4441	CE1	TYR	572	58.623	-7.960	9.936	1.00 30.14
ATOM	4442	CD2	TYR	572	56586	-6.552	11.208	1.00 34.42
ATOM	4443	CE2	TYR	572	56.991	-7.799	11.704	1.00 32.29
MOTA	4444	CZ	TYR	572	58.012	-8.495	11.065	1.00 32.52
ATOM	4445	ОН	TYR	572	58.427	-9.717	11.571	1.00 31.70
MOTA	4447	C	TYR	572	54.588	-5.310	8.754	1.00 37.64
MOTA	4448	0	TYR	572	54.387	-6.410	8.226	1.00 35.70
MOTA	4449	N	LEU	573	53.742	-4.740	9.608	1.00 38.63
MOTA	4451	CA	LEU	573	52.498	-5.376	10.011	1.00 38.21
ATOM	4452	CB	LEU	573	51.802	-4.532	11.067	1.00 35.40
ATOM	4453	CG	LEU	573	52.494	-4.421	12.419	1.00 34.55
MOTA	4454	CD1	LEU	573	51.755	-3.402	13.258	1.00 32.02
MOTA	4455	CD2	LEU	573	52.537	-5.788	13.108	1.00 34.58
MOTA	4456	С	LEU	573	51.570	-5.549	8.818	1.00 38.11
ATOM	4457	0	LEU	573	51.144	-6.656	8.507	1.00 37.68
MOTA	4458	N	GLN	574	51.286	-4.448	8.138	1.00 40.92
MOTA	4460	CA	GLN	574	50.402	-4.476	6.982	1.00 45.16
MOTA	4461	CB	GLN	574	50.213	~3.071	6.447	1.00 44.16
MOTA	4462	CG	GLN	574	49.380	-2.239	7.369	1.00 45.26
ATOM	4463	CD	GLN	574	49.222	-0.849	6.863	1.00 47.09
ATOM	4464	OE1	GLN	574	49.789	-0.483	5.838	1.00 50.83
MOTA	4465	NE2	GLN	574	48.450	-0.051	7.573	1.00 48.95
MOTA	4468	С	GLN	574	50.807	-5.419	5.861	1.00 45.21
MOTA	4469	0	GLN	574	49.951	-6.031	5.215	1.00 49.63
MOTA	4470	N	ALA	575	52.105	-5.562	5.646	1.00 43.35
MOTA	4472	CA	ALA	575	52.579	-6.446	4.604	1.00 42.62
MOTA	4473	CB	ALA	575	54.023	-6.130	4.284	1.00 43.49
ATOM	4474	С	ALA	575	52.439	-7.906	5.022	1.00 42.85
ATOM	4475	0	ALA	575	52.771	-8.804	4.254	1.00 44.43
ATOM	4476	N	ARG	576	51.937	-8.142	6.229	1.00 42.24
ATOM	4478	CA	ARG	576	51.787	-9.494	6.747	1.00 41.58



ATOM 4479 CB ARC S	
ATOM 4400 TO ARG 57	52.813 -9.725 7.015
ATOM 4485 57	6 - 7.849 1 00
ATOM 4422 CD ARG 57	6 55 -9.694 7.314 1 00 1-
ATOM 4482 NE ARG 57	6 55.200 -9.604 8.392 1.00
ATOM 4484 CZ ARG 57	5 7.826 1 00
4485 NU1 350	57.110 -8 604 1.00 41.95
4488 MH2 NDC	56.359 -7.658
4491 0 300	58.347 -8.787
4492 O ARC	50.389 -9.763
ATOM 4493 N 376	50.187 10.55 1.00 43.29
ATOM 4495 CA PRO 577	49 410 - 0.13/ 1.00 43 76
ATOM 4496 CD 577	48.023
ATOM 115	4- /. (// 1 00
ATOM 4400 TO ARG 577	45 - 9.36 ( 1 00
ATOM 4400 CD ARG 577	7.440 1 00
NE ARG Egg	-5.635 6.898 1 00
ATTOM TOTAL CZ. ARG 577	
4502 NH1 ARG	45.750 -3.450 - 1.00 47.76
4505 MH2 305	45.149 -3 225 - 1.00 48.55
4508 C	45.643 -2 560 0.548 1.00 50.64
ATOM 4509 0 377	47.408 -10.540
ATOM 4510 N C	47.396 -10.800 5.603 1.00 47.12
ATOM 4512 CT 594	53 246 73 3.405 1.00 48 27
ATOM 4512 am 594	52.054 12 45 7.891 1.00 64 66
ATOM 4514 C	51 730 34 6.728 1.00 65 10
ATOM 4515 0 GLN 594	51.130 -14.931 6.184 1.00 65.10 52.447 -14.127 16.184 1.00 65.77
ATOM ASSA GLN 594	1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
N LEU SOC	15.201 16.50-
Amore 4518 CA LEU 595	70,103 13,154 11 01 01 01 12
4519 CB LEU 505	32.524 -13.245 12 43-
4520 CG LEU FOR	32.669 -11.826 12 20- 1.00 59.21
4521 ('D) TEST	33.648 -11 <sub>1343</sub> - 2 2 2 2 57.54
4522 CD2 r mr	53.442 -9.551 12 205 4.00 56.37
4523 (1 777)	55.064 -11.430 30 57.06
ATOM 4524 O TR	51.509 -14 046 12.465 1.00 55.57
ATOM 4525 N 000	50 316 13.25/ 1.00 58 34
ATOM 4527 CA 375	52 007 14 - 12.953 1.00 58 21
ATOM 4528 CD 596	57 382 3- 14.280 1.00 58 00
ATOM 4530 - SER 596	51 960 15 13.180 1.00 56 04
ATOM 1532 OG SER 596	21.300 -16.770 15 65-
SER FOR	52.587 -16.403 16 705
' 4332 O SED FOC	
ATOM SER 597	31.473 -13.645 nc == 34.03
4535 CA SER 502	-2.214 -15.133 17 202
4536 CB SEP COR	49.525 -14.389 10.300 56.10
4537 OG SER 507	48.530 -15.196 10 255
4539 C GED 50-	47.620 -15.914 10 405
ATOM 4540 0 500	50.778 -14 004 -18.421 1.00 61.95
ATOM 4541 N 746	50.934 -12 990 1.00 57.75
ATOM 4543 CD THE	51 600 77 13.755 1.00 57 06
ATOM 4544 CD 598	52 930 - +3.2/1 1.00 57 00
ATOM AFAF	53 600 7 20.026 1.00 57 51
ATOM 1515 CG LYS 598	54 470 -16.231 20.124 1.00 57 72
ATOM 4546 CD LYS 598	
454 / CE LVC 500	77.427 -17.724 21 422
4548 NZ 1.VS 500	55.894 -17.989 22 024 1.00 62.23
330	54.921 -18 148 5 1.00 60.79
\$\$\$D/55115	23.949 1.00 61.46

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1.00 55.94 19.389 53.809 -13.829 1.00 55.84 598 LYS 20.089 C 54.322 -12.955 4552 ATOM 1.00 53.32 598 18.061 LYS 0 4553 53.935 -13.866 MOTA 1.00 50.30 599 ASP 17.334 N 54.737 -12.882 4554 MOTA 1.00 49.72 599 ASP 15.823 CA 54.688 -13.119 4556 MOTA 1.00 53.97 599 ASP 15.394 CB 55.426 -14.383 4557 MOTA 1.00 58.12 599 ASP 16.214 CG 56.176 -14 948 4558 MOTA 1.00 55.58 599 OD1 ASP 14.233 55.261 -14.822 4559 MOTA 1.00 49.53 599 OD2 ASP 17.636 54.247 -11.474 4560 MOTA 599 1.00 51.16 ASP C 17.911 55.054 -10.589 4561 ATOM 599 1.00 47.50 ASP 0 17.634 52.930 -11.281 4562 MOTA 1.00 45.41 600 LEU 17.909 N 4563 -9.972 MOTA 52.354 1.00 43.77 600 1.7.627 LEU CA ..9.948 4565 MOTA 50.850 1.00 41.05 600 LEU 16.169 4566 CB 50.429 -10.121 MOTA 1.00 41.04 600 LEU 16.048 4567 CG -9 904 48.941 MOTA 600 1.00 39.59 CD1 LEU 15.294 4568 -9 140 MOTA 51.160 1.00 46.77 600 CD2 LEU 19.318 4569 -9.485 MOTA 52.638 1.00 48.74 600 LEU C 19.497 4570 ~B.308 MOTA 52.964 1.00 47.64 600 LEU 20 314 0 52.524 -10.372 4571 MOTA 1.00 47.38 601 VAL 21.716 4572 И 52.804 -10.002 MOTA 1.00 46.58 601 VAL CA 22.756 4574 52.321 -11.070 MOTA 1.00 45.07 601 VAL 24.114 CB 52.081 -10.403 4575 MOTA 1.00 48.86 601 CG1 VAL 22.306 4576 51.058 -11.759 MOTA 1.00 46.04 601 21.890 CG2 VAL 4577 -9.811 MOTA 54.321 1.00 46.13 601 VAL 22.622  $\mathbf{C}$ -8.935 4578 MOTA 54.793 1.00 44.21 601 JAV 21.183 Ü 4579 55.090 -10.624 ATOM 1.00 42.78 602 21.233 SER N 4580 56.534 -10.546 ATOM 1.00 43.98 602 SER 20,297 4582 CA 57.119 -11.594 MOTA 1.00 51.02 602 SER CB 20.355 58.523 -11.615 4583 ATOM 602 1.00 41.74 SER 20.813 OG 4584 -9.135 MOTA 56.954 1.00 44.09 602 21.524 SER C 4586 -8.467 ATOM 57.709 1.00 39.57 602 SER 19.685 4587 0 -B.667 ATOM 56.425 1.00 36.11 603 CYS 19.177 4588 N -7.317 MOTA 56.699 1.00 34.72 603 CYS 17.924 CA -7.058 4590 MOTA 55.852 0.50 29.10 PRT1 603 CYS CB 17.323 4591 -5.364 MOTA 55.760 1.00 34.50 603 CYS 20.252 SG 4592 -6.272 MOTA 56.378 1.00 33.61 603 C CYS 20.506 4593 -5.371 MOTA 57.174 1.00 34.64 603 CYS 20.913 0 4594 -6.429 MOTA 55.236 1.00 37.18 604 ALA N -5.50€ 21.964 4595 MOTA 54.811 1.00 38.20 604 ALA CA -5.850 22.414 4597 MOTA 53.386 604 1.00 38.91 ALA 4598 CB 23.160 MOTA -5.516 55.786 1.00 38.29 604 ALA 23.790 4599 C -4.481 MOTA 56.026 1.00 39.54 604 ALA 23.477 0 4600 -6.693 MOTA 56.323 1.00 39.29 605 24.565 TYR N 4601 -6.854 MOTA 57.283 1.00 40.07 605 TYR 24.791 CA 4603 -8.340 MOTA 57.573 605 1.00 39.09 TYR CB 25.807 4604 -8.622 MOTA 58.663 1.00 38.50 605 TYR CG 27.137 4605 -8.236 MOTA 58.525 1.00 40.76 605 CD1 TYR 28.074 4606 -8.505 MOTA 59.526 1.00 39.73 605 CE1 TYR 25.435 4607 -9.283 MOTA 59.831 1.00 37.45 605 CD2 TYR 26.361 4608 -9.553 MOTA 60.834 1.00 40.34 CE2 TYR 605 4609 27.677 ATOM -9.166 60.678 1.00 43.16 605 TYR 28.601 CZ4610 ATOM -9.466 61.666 605 TYR OH 4611 ATOM

ATO	1 1612	_		
ATON	-013	C TYR		
ATOM		O TYR		59 067 - 24.224 1.00 39 45
ATOM		N GLN	606	59 120 - 25.022 1.00 38 75
ATOM		CA GLN	606	60 361 - 23.040 1.00 36 41
ATOM		CB GLN	606	22.550 1 00 35 35
ATOM	1019	CG GLN	606	21.150 1 00 34 0
ATOM	4620	CD GLN	606	51.286 -7.695 21.118 1 00 22 2
ATOM	4621	OE1 GLN	606	51.302 -8.205 19.709 1 00 32.21
ATOM	4622	NE2 GLN	606	02.495 -7.888 19.075 1.00 32.63
		C GLN	606	00.368 -9.004 19.216 1.00 34.40
ATOM		O GLN	606	60.286 -4.252 22.525 1 00 36 00
ATOM		VAL	607	51.209 -3.572 22.989 1 00 38 5
ATOM		CA VAL	607	33.108 -3.716 21.998 1.00 22
ATOM		B VAL	607	58.979 -2.280 21 923
АТОМ	4631 (	G1 VAL	607	57.651 -1.948 21 190
ATOM	4632 C	G2 VAL	607	57.260 -0.495 21 401
ATOM	4633 C		607	57.790 -2.244 19.600
ATOM	4634 C		607	58.965 -1.698 22 222
ATOM	4635 N		608	59.557 -0.643 22 570
ATOM	4637 C			58.317 -2.402 24 270 -1.00 33.86
MOTA	4638 CE		608	58.235 -1.971 25 667
ATOM	4639 C	ALA	608	57.255 -2.836 26.440 1.00 28.98
ATOM	4640 O		608	59.598 -1.979 26 353
ATOM	4641 N	3.5-	608	59.889 -1.091 27.155
ATOM	4643 CA	<b>3</b>	609	60,435 -2,959 36 639
ATOM	4644 CB	7.20	609	51.765 -3.023 26.032 1.00 28.79
	4645 CG	77-	609	62.499 -4 301 - 1.00 30.90
ATOM	4646 CD	350	509	51.787 -5.571 26 527
ATOM	4647 NE		509	62.782 -6 707 0- 1.00 41.94
ATOM .	1649 CZ	***	509	63.392 -6 93, 1.00 44.70
ATOM			09	64.4447 500 1.00 47.13
7 177014	653 NH2	355	09	65.025 .9 314 1.00 48.71
A mos.	656 C		09	64.897 -7 655 1.00 48.33
ATOM 4	657 0		09	62.602 -1 915 1.00 49.11
ATOM 4	658 N	_	09	63.215 -1.140 1.00 32.38
7 more	660 CA		10	62.636 -1 554 27.058 1.00 32.63
7.000	661 C	G=		63.3840 430 29.98
3	662 0	~		62.969 0 937 2 1.00 25.65
N DDC 14				63,791 1 640 1.00 25.44
ATOM 46		MET 61		61.672 1.009 25.2463 1.00 27.09
		MET 61	_	61.167 2.176 25.242 1.00 30.41
	C -	MET 61		59.653 2 222 23.543 1.00 31.34
3	CO -	MET 61		59.195 3.505 23.832 1.00 28.39
ATOM 46	· · · ·	MET 61		59.904 4 182 24.449 1.00 25.17
ATOM 46	70 -	MET 61:		59.458 5 150 24.005 1.00 26.65
ATOM 46	73 -	MET 611		61.600 2.176 25.453 1.00 19.78
ATOM 46		MET 611		62.008 3 311 27.412 1.00 34.05
ATOM 46	, ,	LU 612		61.500 1.006 1.00 33.79
7 mos-		LU 612		61.893 0.013 28.078 1.00 37.16
ATOM 467		LU 612		61 733 29.484 1.00 38 85
3 77014	•	LU 612	é	62 340 - 29.988 1.00 38 96
B.Moss	0.	LU 612		52 316 31,400 1.00 35 19
ATOM 467	8 OEl G	LU 612	è	52 605 21.783 1.00 35 26
				52.605 -3.123 30.912 1.00 29.29
SSSD/55145	21			

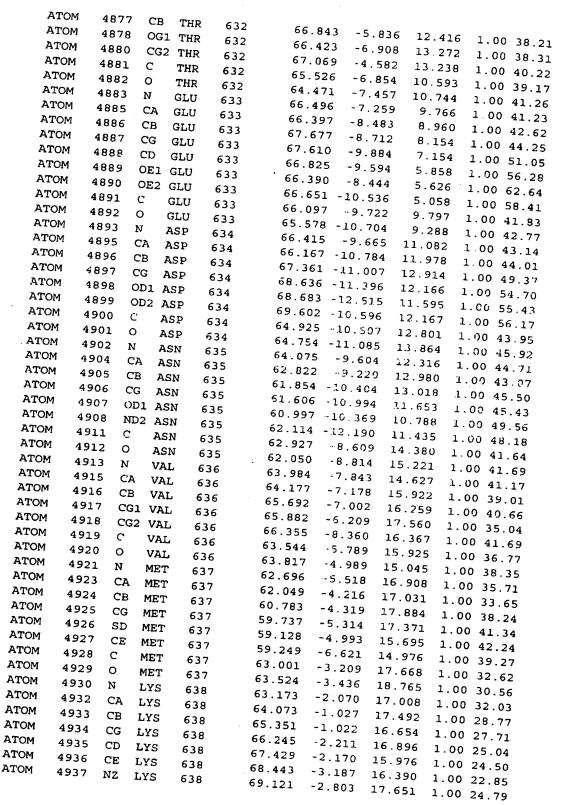
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ATOM	4679	OE2	GLU	612	62.102	-2.588	32.982	1.00	37.85
MOTA	4680	С	GLU	612	63.353	1.364	29.628	1.00	40.01
ATOM	4681	0	GLU	612	63.720	2.060	30.584	1.00	38.27
ATOM	4682	N	TYR	613	64.176	0.972	28.662	1.00	40.33
ATOM	4684	CA	TYR	613	65.575	1.362	28.664	1.00	39.71
ATOM	4685	CB	TYR	613	66.333	0.722	27.494	1.00	39.03
ATOM	4686	CG	TYR	613	67.800	1.100	27.467	1.00	41.41
ATOM	4687	CD1	TYR	613	68.702	0.527	28.364	1.00	42.79
MOTA	4688	CE1	TYR	613	70.048	0.905	28.386	1.00	40.21
ATOM	4689	CD2	TYR	613	68.283	2.068	26.581	1.00	39.75
MOTA	4690	CE2	TYR	613	69.621	2.454	26.596	1.00	39.01
ATOM	4691	CZ	TYR	613	70.499	1.868	27.503	1.00	39.56
ATOM	4692	OH	TYR	613	71.823	2.249	27.538	1.00	35.63
MOTA	4694	C	TYR	613	65.642	2.881	28.562	1.00	38.71
ATOM	4695	0	TYR	613	66.106	3.541	29.486	1.00	38.52
MOTA	4696	N	LEU	614	65.126	3.423	27.460	1.00	37.22
ATOM	4698	CA	LEU	614	65.128	4.864	27.212	1.00	35.66
ATOM	4699	CB	LEU	614	64.223	5.202	26.025	1.00	35.27
MOTA	4700	CG	LEU	614	64.687	4.699	24.659	1.00	33.09
ATOM	4701	CD1	LEU	614	63.718	5.188	23.612	1.00	33.31
MOTA	4702	CD2	LEU	614	66.099	5.184	24.363	1.00	31.20
ATOM	4703	C	LEU	614	64.672	5.653	28.430	1.00	35.64
ATOM	4704	0	LEU	614	65.298	6.639	28.816	1.00	34.54
ATOM	4705	N	ALA	615	63.577	5.203	29.032	1.00	36.61
ATOM	4707	CA	ALA	615	63.028	5.835	30.222	1.00	37.74
ATOM	4708	CB	ALA	615	61.682	5.187	30.608	1.00	37.74
MOTA	4709	С	ALA	615	64.021	5.776	31.389	1.00	37.30
MOTA	4710	0	ALA	615	64.111	6.731	32.175	1.00	37.29
MOTA	4711	И	SER	616	64.752	4.665	31.511	1.00	37.18
ATOM	4713	CA	SER	616	65.741	4.534	32.577	1.00	36.92
ATOM	4714	CB	SER	616	66.274	3.091	32.702		34.82
ATOM	4715	OG	SER	616	67.106	2.680	31.628	1.00	28.79
ATOM	4717	C	SER	616	66.870	5.516	32.287		38.57
ATOM	4718	0	SER	616	67.633	5.902	33.179		38.30
MOTA	4719	N	LYS	617	66.958	5.925	31.024		37.62
MOTA	4721	CA	LYS	617	67.965	6.876	30.606		36.13
ATOM	4722	CB	LYS	617	68.511	6.494	29.238		35.90
ATOM	4723	CG	LYS	617	69.274	5.206	29.236		34.58
ATOM	4724	CD	LYS	617	70.502	5.348	30.077		35.44
ATOM	4725	CE	LYS	617	71.201	4.022	30.232		38.54
ATOM	4726	NZ	LYS	617	72.566	4.211	30.790		41.54
ATOM	4730	С	LYS	617	67.378	8.275	30.564		36.55
ATOM	4731	0	LYS	617	67.943	9.155	29.934		40.26
ATOM	4732	N	LYS	618	66.221	8.468	31.187		36.42
ATOM	4734	CA	LYS	618	65.570	9.779	31.231		36.06
ATOM	4735	СВ	LYS	618	66.543	10.833	31.746		42.22
ATOM	4736	CG	LYS	618	67.234	10.499	33.062		52.36
ATOM	4737	CD	LYS	618	66.301	10.668	34.236		61.51
ATOM	4738	CE	LYS	618	66.933	10.121	35.495		67.28
ATOM	4739	NZ	LYS	618	65.965	10.161	36.618		73.99
ATOM	4743	C	LYS	618	65.026	10.261	29.887		34.94
ATOM	4744	0	LYS	618	64.562	11.393	29.781	1.00	34.69

3.000	_							
ATO		N CYS	619	a-				
ATON	,	CA CYS	619	05.	.051	9.407 2	8.872	2 00 2
ATOM	4/40	CB CYS	619	64.	588 9		7.543	1.00 34.46
ATOM	4749	SG CYS			311 8		6.475	1.00 33.12
ATOM	4 7 7 4	C CYS	619	64.	920 9		4.778	1.00 34.33
ATOM	4255	_	619	63.				1.00 35.64
ATOM	4750		619	62.4			7.355	1.00 32.13
ATOM	4754		620	62.4			584	1.00 30.72
ATOM	4755	CA ILE	620	61.0	_		.960	1.00 32.70
ATOM		B ILE	620	60.4			.708	1.00 32.75
ATOM		G2 ILE	620	59.0		129 27	.421	1.00 33.55
ATOM		G1 ILE	620	60.4			. 986	1.00 38.39
ATOM	4555	D1 ILE	620	59.9			. 933	1.00 30.71
ATOM	4759 C	ILE	620	60 0		084 29	710	1.00 30.11
ATOM	4760 O	ILE	620	60.96		086 25	_	1.00 33.31
	4761 N	777	621	61.51		040 24	_	L.00 33.40
ATOM	4763 CA	٠	621	60.35		114 24.		
ATOM	4764 CB		521	60.23	30 10.0			.00 33.56
ATOM	4765 CG			59.86	6 8.6			.00 32.30
ATOM	4766 CD	` ·	521	60.04	9 8.4			.00 29.55
ATOM	4767 ND	3 ***·	21	60.69	4 7.4			.00 27.32
ATOM	4769 CE	_	21	59.46	2 9. <sub>1</sub>			.00 24.26
ATOM	4770 NE	· · · · ·	21	59.734	4 8.6			.00 25.20
ATOM	4772 C		21	60.48]	7.5			.00 25.81
ATOM	4773 U		21	59.246	5 11.10			00 26.65
ATOM	4774 N		21	59.459			99 1.	00 35.40
ATOM	470-		22	58.128	11.36		88 1.	00 39.18
ATOM	475-		22	57.117			78 <u>I</u> .	00 36.39
A COOL	4:70-	ARG 62	22	57.694	_		36 <u>1</u> .	00 36.40
30000	4754	ARG 62	2	58.171			17 1.	00 35.62
<b>\ m</b> =	1700	ARG 62	2	58.837			37 1.0	00 33.79
3	1780 NE	ARG 62	2	59,315	15.59	-	9 0.5	30 32.17
A CONT	782 CZ	ARG 62	2	60.487	16.10		2 0.5	32.82
•	783 NH1	ARG 62	2	61 336	15.786		5 0.5	0 34.07
7 mose	786 NH2	ARG 62:		61.326	14.965		2 0.5	0 33.44
	789 C	ARG 622		60,803	16.268	26.76	_	0 32.70
	790 Ö	ARG 622		56.405	12.008	21.35		0 36.23
	791 N	ASP 623		55.527	12.763	20.936		0 36.23
	793 CA 1	ASP 623		56.806	10.938	20.668	_	
	<sup>794</sup> CB 2	ASP 623		56.128	10.538	19.436		0 35.84
ATOM 4	705	ASP 623		56.574	11.352	18.221		35.68
ATOM 4		LSP 623		55.736	11.036	16.974		38.71
ATOM 4	97 OD2 A			56.277	11.082	15.851		46.29
ATOM 47				54.535	10.715	17.119	1.00	52.33
	^-			56.271	9.052			50.45
ATOM 48	00	SP 623		56.664	8.645	19.162	1.00	32.98
ATOM 48		EU 624		56.015	8.244	18.073	1.00	30.90
ATOM 48	00	EU 624		56.099	6 001	20.179	1.00	31.16
ATOM 48		EU 624		56.070	6.801	20.029	1.00	31.71
A moss		EU 624		56.049	6.144	21.407	1.00	28.48
		EU 624		57.225	4.618	21.514	1.00	28.13
T.Mossa		U 624		56.072	3.975	20.799	1.00	27.00
30000				E 4 0 2 -	4.283	22.987	1.00	29.10
			-		6.320	19.185	1.00	32 62
ATOM 480	9 N AL		-		6.608	19.508	1.00	J4.0/
		~ J	5	55.214		18.081	1 00	33.74
SSSD/55145						. =	1.00	49.82

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ATOM 4811 CA ALA 625 54.194 5.106 17.181 1.00 28.29 ATOM 4813 C ALA 625 53.682 6.182 16.245 1.00 26.27 ATOM 4813 C ALA 625 54.895 4.031 16.395 1.00 28.40 ATOM 4815 N ALA 625 54.895 4.031 16.395 1.00 28.40 ATOM 4815 N ALA 626 54.131 3.135 15.770 1.00 28.55 ATOM 4818 CB ALA 626 54.687 2.028 14.979 1.00 28.55 ATOM 4818 CB ALA 626 54.687 2.028 14.979 1.00 26.25 ATOM 4819 C ALA 626 55.569 2.573 13.892 1.00 23.68 ATOM 4820 O ALA 626 55.569 2.573 13.892 1.00 23.68 ATOM 4821 N ARG 627 55.208 3.744 13.378 1.00 23.80 ATOM 4823 CA ARG 627 55.208 3.744 13.378 1.00 23.80 ATOM 4824 CB ARG 627 55.289 5.728 11.914 1.00 25.57 ATOM 4825 CG ARG 627 54.991 6.692 13.055 1.00 23.60 ATOM 4826 CD ARG 627 54.711 8.130 12.584 1.00 23.80 ATOM 4827 NE ARG 627 54.260 8.978 13.691 1.00 34.18 ATOM 4828 ARG 627 55.208 3.744 0.91 1.00 34.18 ATOM 4829 CZ ARG 627 54.260 8.978 13.691 1.00 34.18 ATOM 4828 ARG 627 54.260 8.978 13.691 1.00 34.18 ATOM 4829 CZ ARG 627 52.097 9.067 14.091 1.00 35.88 ATOM 4831 NHZ ARG 627 52.689 9.748 15.183 1.00 29.24 ATOM 4833 NHZ ARG 627 52.689 9.748 15.183 1.00 29.23 ATOM 4831 N ARG 627 52.689 9.748 15.183 1.00 29.24 ATOM 4838 N ASN 628 57.634 4.938 11.007 1.00 29.24 ATOM 4831 N ARG 627 56.369 1.00 29.03 ATOM 4831 N ASN 628 58.864 5.359 15.676 1.00 29.51 ATOM 4841 CB ASN 628 58.864 5.359 15.676 1.00 29.51 ATOM 4843 CA ASN 628 58.864 5.359 15.676 1.00 29.51 ATOM 4844 NDZ ASN 628 58.864 6.359 15.676 1.00 29.32 ATOM 4848 CA ASN 628 58.859 7.639 15.225 1.00 25.73 ATOM 4848 CA ASN 628 58.859 7.639 15.225 1.00 25.73 ATOM 4848 CA ASN 628 58.859 7.639 15.225 1.00 25.73 ATOM 4848 CA ASN 628 59.684 0.339 15.225 1.00 25.73 ATOM 4848 CA ASN 628 59.684 0.339 15.225 1.00 25.73 ATOM 4848 CA ASN 628 59.684 0.339 15.225 1.00 25.73 ATOM 4848 CA ASN 628 59.684 0.339 15.225 1.00 25.73 ATOM 4848 CA ASN 628 59.684 0.339 15.225 1.00 25.73 ATOM 4859 CA ASN 628 59.684 1.00 15.315 1.00 28.60 ATOM 4851 CA VAL 629 59.826 1.600 11.900 2.798 ATOM 4860 CA ASN 628 59.694 2.0004 11.00 20.279 ATOM 4861 CA ASN 628 59.684 1.000 11.00 20.279 ATOM 4864	A TIOM	4033	~ n	212	C25	C4 204	E 100	17 101	1 00 00 00
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ATOM 4818 CB ALA 626 53.577 1.169 14.365 1.00 23.54 ATOM 4819 C ALA 626 55.569 2.573 13.892 1.00 23.54 ATOM 4820 O ALA 626 55.569 2.573 13.892 1.00 23.60 ATOM 4821 N ARG 627 55.208 3.744 13.378 1.00 26.07 ATOM 4823 CA ARG 627 55.980 4.413 12.338 1.00 26.57 ATOM 4824 CB ARG 627 55.980 4.413 12.338 1.00 26.57 ATOM 4825 CG ARG 627 55.980 4.413 12.338 1.00 25.91 ATOM 4826 CD ARG 627 54.991 6.692 13.055 1.00 27.60 ATOM 4827 NE ARG 627 54.991 6.692 13.055 1.00 27.60 ATOM 4828 CZ ARG 627 54.991 6.692 13.055 1.00 27.60 ATOM 4829 CZ ARG 627 54.991 8.3691 1.00 34.18 ATOM 4830 NH1 ARG 627 52.997 9.067 14.091 1.00 35.88 ATOM 4830 NH1 ARG 627 52.056 8.380 13.460 1.00 38.89 ATOM 4833 NH2 ARG 627 52.056 8.380 13.460 1.00 36.43 ATOM 4836 C ARG 627 57.439 4.686 12.785 1.00 29.24 ATOM 4838 N ASN 628 57.634 4.938 14.087 1.00 29.51 ATOM 4840 CA ASN 628 58.362 4.606 11.972 1.00 29.24 ATOM 4840 CA ASN 628 58.954 5.234 14.645 1.00 29.51 ATOM 4841 CB ASN 628 58.954 5.234 14.645 1.00 29.13 ATOM 4842 CG ASN 628 58.539 7.687 15.035 1.00 29.51 ATOM 4843 ODI ASN 628 58.539 7.687 15.035 1.00 29.51 ATOM 4844 NDZ ASN 628 59.079 8.028 13.999 1.00 32.09 ATOM 4848 N VAL 629 59.898 13.699 1.00 22.79 ATOM 4849 N VAL 629 59.898 16.601 15.315 1.00 27.78 ATOM 4850 C ALC 629 59.828 16.600 15.315 1.00 22.96 ATOM 4851 CA VAL 629 59.828 16.600 15.315 1.00 22.96 ATOM 4851 CA VAL 629 59.828 16.600 15.315 1.00 22.96 ATOM 4854 CG VAL 629 59.492 -0.604 16.412 1.00 26.63 ATOM 4855 C VAL 629 59.492 -0.604 16.412 1.00 26.95 ATOM 4856 C VAL 629 59.492 -0.604 16.412 1.00 26.95 ATOM 4865 C VAL 629 59.494 11.972 1.00 11.86 ATOM 4866 N VAL 631 62.626 -0.021 12.665 1.00 29.74 ATOM 4866 C RU CAL 631 62.626 -0.021 12.665 1.00 29.74 ATOM 4867 N LEU 630 62.627 -0.021 12.665 1.00 29.74 ATOM 4868 CA VAL 631 62.626 -0.021 12.665 1.00 29.74 ATOM 4869 CB VAL 631 62.626 -0.021 12.665 1.00 19.25 ATOM 4860 CB LEU 630 62.627 -0.021 12.665 1.00 29.74 ATOM 4860 CD LEU 630 62.627 -0.021 12.665 1.00 31.75 ATOM 4860 CD VAL 631 62.646 -3.790 10.00 71.00 31.75 ATOM 4861 CD LEU 630 62.627									
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ATOM 4820 O ALA 626 56.544 1.944 13.519 1.00 26.07 ATOM 4821 N ARG 627 55.208 3.744 13.378 1.00 23.6.07 ATOM 4823 CA ARG 627 55.208 3.744 13.378 1.00 23.6.57 ATOM 4824 CB ARG 627 55.980 4.413 12.338 1.00 25.57 ATOM 4825 CG ARG 627 55.980 5.728 11.914 1.00 25.91 ATOM 4826 CD ARG 627 54.991 6.692 13.055 1.00 27.60 ATOM 4827 NE ARG 627 54.991 6.692 13.055 1.00 27.60 ATOM 4828 CD ARG 627 54.991 6.692 13.055 1.00 27.60 ATOM 4829 CZ ARG 627 54.911 8.130 12.584 1.00 34.18 ATOM 4830 NH1 ARG 627 52.997 9.067 14.091 1.00 35.88 ATOM 4830 NH1 ARG 627 52.056 8.380 13.460 1.00 36.43 ATOM 4833 NH2 ARG 627 52.056 8.380 13.460 1.00 36.43 ATOM 4836 C ARG 627 57.439 4.686 12.785 1.00 29.03 ATOM 4838 N ASN 628 58.624 4.636 11.972 1.00 29.24 ATOM 4838 N ASN 628 58.644 4.938 14.087 1.00 29.51 ATOM 4840 CA ASN 628 58.954 5.234 14.645 1.00 26.41 ATOM 4841 CB ASN 628 58.954 5.234 14.645 1.00 26.41 ATOM 4841 CB ASN 628 58.539 7.687 15.076 1.00 25.32 ATOM 4842 CG ASN 628 58.539 7.687 15.075 1.00 29.37 ATOM 4848 N ASN 628 58.539 7.687 15.075 1.00 25.32 ATOM 4848 N ASN 628 58.539 8.028 13.999 1.00 32.09 ATOM 4848 N DZ ASN 628 59.079 8.028 13.999 1.00 32.09 ATOM 4848 N DZ ASN 628 59.684 4.039 15.225 1.00 25.77 ATOM 4848 N VAL 629 59.209 2.853 14.874 1.00 26.61 ATOM 4855 CD VAL 629 59.828 1.610 15.315 1.00 25.34 ATOM 4855 CD VAL 629 59.828 1.610 15.315 1.00 25.34 ATOM 4855 CD VAL 629 59.828 1.610 15.315 1.00 22.96 ATOM 4857 N LEU 630 62.062 -0.021 12.685 1.00 22.96 ATOM 4860 CB LEU 630 62.062 -0.021 12.685 1.00 22.99 ATOM 4861 CG LEU 630 62.062 -0.021 12.685 1.00 22.99 ATOM 4862 CD LEU 630 62.367 -1.492 12.961 1.00 22.99 ATOM 4863 CD LEU 630 62.267 -1.492 12.961 1.00 22.95 ATOM 4866 C VAL 631 63.697 -4.286 11.305 1.00 31.75 ATOM 4867 C LEU 630 62.267 -1.492 12.961 1.00 22.95 ATOM 4868 CA VAL 631 63.697 -4.286 11.305 1.00 31.75 ATOM 4868 CA VAL 631 63.697 -4.286 11.305 1.00 31.75 ATOM 4867 C LEU 630 62.267 -1.492 12.961 1.00 22.95 ATOM 4868 CA VAL 631 63.697 -4.286 11.305 1.00 30.04 ATOM 4867 C LEU 630 62.266 -3.790 12.098 1.00 31.75 ATOM 486	ATOM	4818			626	53.577	1.169	14.365	1.00 23.54
ATOM 4821 N ARG 627 55.208 3.744 13.378 1.00 23.80 ATOM 4823 CA ARG 627 55.980 4.413 12.338 1.00 25.91 ATOM 4824 CB ARG 627 55.289 5.728 11.914 1.00 25.91 ATOM 4825 CG ARG 627 54.991 6.692 13.055 1.00 27.60 ATOM 4827 NE ARG 627 54.791 8.130 12.584 1.00 33.01 ATOM 4827 NE ARG 627 54.260 8.978 13.691 1.00 34.18 ATOM 4829 CZ ARG 627 54.260 8.978 13.691 1.00 34.18 ATOM 4830 NH1 ARG 627 52.997 9.067 14.091 1.00 35.88 ATOM 4830 NH1 ARG 627 52.056 8.380 13.466 1.00 38.89 ATOM 4831 NH2 ARG 627 52.699 9.748 15.183 1.00 29.03 ATOM 4833 NH2 ARG 627 52.689 9.748 15.183 1.00 29.03 ATOM 4831 NA ARG 627 58.362 4.606 12.785 1.00 29.24 ATOM 4836 C ARG 627 58.362 4.606 12.785 1.00 29.24 ATOM 4838 N ASN 628 57.634 4.938 14.087 1.00 29.51 ATOM 4841 CB ASN 628 58.954 5.234 14.645 1.00 26.41 ATOM 4842 CG ASN 628 58.954 5.234 14.645 1.00 26.41 ATOM 4843 OD1 ASN 628 57.634 4.036 11.972 1.00 29.21 ATOM 4844 ND2 ASN 628 58.539 7.687 15.035 1.00 28.11 ATOM 4844 ND2 ASN 628 58.539 7.687 15.035 1.00 28.11 ATOM 4844 ND2 ASN 628 59.079 8.028 13.999 1.00 32.09 ATOM 4849 N VAL 629 59.209 2.853 14.874 10.00 25.77 ATOM 4849 N VAL 629 59.209 2.853 14.874 10.00 25.77 ATOM 4855 C VAL 629 59.828 1.610 15.315 1.00 22.94 ATOM 4855 C VAL 629 59.492 -0.604 16.412 1.00 22.95 ATOM 4854 CG VAL 629 59.492 -0.604 16.412 1.00 22.95 ATOM 4853 CG1 VAL 629 59.492 -0.604 16.412 1.00 22.97 ATOM 4854 CG2 VAL 629 59.492 -0.604 16.412 1.00 22.97 ATOM 4855 C VAL 629 59.492 -0.604 16.412 1.00 22.97 ATOM 4856 O VAL 629 59.492 -0.604 16.412 1.00 22.97 ATOM 4857 N LEU 630 63.297 -0.733 12.210 1.00 22.79 ATOM 4863 CD2 LEU 630 62.367 -1.492 12.961 1.00 22.95 ATOM 4864 C LEU 630 62.266 0.962 14.007 1.00 26.79 ATOM 4865 C VAL 629 59.454 0.839 13.087 1.00 25.91 ATOM 4866 N VAL 631 63.648 -3.790 12.098 1.00 31.75 ATOM 4868 CA VAL 631 63.649 -3.999 10.009 1.00 31.75 ATOM 4868 CA VAL 631 63.649 -3.999 10.009 1.00 32.09 ATOM 4868 CA VAL 631 63.649 -3.999 10.009 1.00 24.59 ATOM 4870 CG1 VAL 631 63.849 -3.999 10.009 1.00 24.59 ATOM 4873 O VAL 631 63.849 -3.999 10.009 1.00 36.24	ATOM	4819	С	ALA	626	55.569	2.573	13.892	1.00 23.68
ATOM 4823 CA ARG 627 55.980 4.413 12.338 1.00 26.57 ATOM 4825 CG ARG 627 55.289 5.728 11.914 1.00 25.91 ATOM 4825 CG ARG 627 54.991 6.692 13.055 1.00 27.60 ATOM 4826 CD ARG 627 54.991 8.130 12.584 1.00 33.01 ATOM 4827 NE ARG 627 54.260 8.978 13.691 1.00 33.01 ATOM 4829 CZ ARG 627 52.997 9.067 14.091 1.00 35.88 ATOM 4830 NH1 ARG 627 52.997 9.067 14.091 1.00 35.88 ATOM 4830 NH1 ARG 627 52.056 8.380 13.460 1.00 29.03 ATOM 4837 O ARG 627 52.689 9.748 15.183 1.00 26.43 ATOM 4838 C ARG 627 52.689 9.748 15.183 1.00 29.03 ATOM 4837 O ARG 627 57.439 4.686 12.785 1.00 29.03 ATOM 4838 N ASN 628 57.634 4.938 14.087 1.00 29.03 ATOM 4840 CA ASN 628 58.954 5.234 14.645 1.00 29.51 ATOM 4840 CA ASN 628 58.954 5.234 14.645 1.00 26.41 ATOM 4841 CB ASN 628 58.864 6.359 15.676 1.00 25.32 ATOM 4842 CG ASN 628 58.589 7.687 15.035 1.00 28.11 ATOM 4843 OUJ ASN 628 58.589 7.687 15.035 1.00 22.09 ATOM 4844 ND2 ASN 628 59.079 8.028 13.999 1.00 32.09 ATOM 4844 ND2 ASN 628 59.699 8.028 13.999 1.00 22.09 ATOM 4848 O ASN 628 59.699 8.028 13.999 1.00 22.09 ATOM 4848 O ASN 628 59.699 8.028 13.999 15.00 25.77 ATOM 4848 O ASN 628 59.699 8.028 15.676 1.00 25.34 ATOM 4848 CO ASN 628 59.684 4.039 15.225 1.00 25.77 ATOM 4848 CO ASN 628 60.641 4.188 16.001 1.00 24.77 ATOM 4848 CO ASN 628 60.641 4.188 16.001 1.00 22.96 ATOM 4851 CA VAL 629 59.209 2.853 14.874 1.00 26.63 ATOM 4852 CB VAL 629 59.828 1.610 15.315 1.00 25.34 ATOM 4853 CGI VAL 629 59.492 -0.604 16.412 1.00 22.96 ATOM 4854 CG2 VAL 629 59.492 -0.604 16.017 1.00 26.65 ATOM 4855 C VAL 629 59.492 -0.604 16.017 1.00 26.95 ATOM 4856 O VAL 629 59.492 -0.604 16.012 1.00 22.96 ATOM 4857 N LEU 630 62.662 -0.021 12.685 1.00 25.91 ATOM 4868 CG VAL 629 59.494 0.839 13.087 1.00 28.60 ATOM 4869 CB VAL 630 62.662 -0.021 12.685 1.00 22.99 ATOM 4866 N VAL 631 63.697 -1.492 12.996 1.00 28.26 ATOM 4867 CG LEU 630 62.367 -1.492 12.996 1.00 28.26 ATOM 4868 CA VAL 631 62.468 -3.790 12.098 1.00 31.75 ATOM 4869 CB VAL 631 62.468 -3.790 12.098 1.00 24.59 ATOM 4870 CGI VAL 631 63.849 -3.999 10.007 1.00 24.59 ATOM 4870	MOTA	4820	О	ALA	626	56.544	1.944	13.519	1.00 26.07
ATOM 4824 CB ARG 627 55.289 5.728 11.914 1.00 25.91 ATOM 4825 CG ARG 627 54.991 6.692 13.055 1.00 27.60 ATOM 4826 CD ARG 627 54.991 8.13.051 1.00 33.01 ATOM 4827 NE ARG 627 54.791 8.130 12.584 1.00 33.01 ATOM 4829 CZ ARG 627 52.997 9.067 14.091 1.00 34.18 ATOM 4830 NH1 ARG 627 52.056 8.380 13.460 1.00 34.18 ATOM 4831 NH2 ARG 627 52.689 9.748 15.183 1.00 36.43 ATOM 4833 NH2 ARG 627 52.689 9.748 15.183 1.00 29.03 ATOM 4837 O ARG 627 58.362 4.606 12.785 1.00 29.03 ATOM 4838 N ASN 628 57.634 4.938 14.087 1.00 29.51 ATOM 4840 CA ASN 628 58.954 5.234 14.645 1.00 26.41 ATOM 4841 CB ASN 628 58.894 5.339 15.676 1.00 25.32 ATOM 4842 CG ASN 628 58.539 7.687 15.035 10.00 22.18 ATOM 4844 ND2 ASN 628 59.079 8.028 13.999 1.00 32.09 ATOM 4848 O ASN 628 57.634 4.038 13.999 1.00 32.09 ATOM 4848 O ASN 628 59.079 8.028 13.999 1.00 22.78 ATOM 4848 ND ASN 628 59.684 4.039 15.225 1.00 25.78 ATOM 4848 O ASN 628 59.684 4.039 15.225 1.00 25.78 ATOM 4848 O ASN 628 59.684 4.039 15.225 1.00 25.78 ATOM 4848 O ASN 628 59.684 4.039 15.225 1.00 25.78 ATOM 4849 N VAL 629 59.288 1.610 15.315 1.00 24.77 ATOM 4851 CA VAL 629 59.828 1.610 15.315 1.00 22.96 ATOM 4851 CA VAL 629 59.828 1.610 15.315 1.00 22.96 ATOM 4853 CGI VAL 629 59.828 1.610 15.315 1.00 22.96 ATOM 4854 CG2 VAL 629 59.492 -0.604 16.412 1.00 22.96 ATOM 4855 C VAL 629 59.492 -0.604 16.412 1.00 22.96 ATOM 4857 N LEU 630 63.297 0.733 12.210 1.00 22.79 ATOM 4860 CB LEU 630 63.297 0.733 12.210 1.00 22.79 ATOM 4860 CB LEU 630 63.297 0.733 12.210 1.00 22.79 ATOM 4860 CB LEU 630 63.297 0.733 12.210 1.00 22.79 ATOM 4860 CB LEU 630 62.629 -1.852 14.101 1.00 28.66 ATOM 4860 CB LEU 630 62.629 -1.852 14.101 1.00 28.66 ATOM 4860 CB LEU 630 62.629 -1.852 14.101 1.00 28.06 ATOM 4860 CB LEU 630 62.629 -1.852 14.101 1.00 28.06 ATOM 4860 CB LEU 630 62.629 -1.852 14.101 1.00 28.06 ATOM 4860 CB LEU 630 62.629 -1.852 14.101 1.00 29.25 ATOM 4860 CB LEU 630 62.629 -1.852 14.101 1.00 20.04 ATOM 4860 CB VAL 631 62.468 -3.790 12.098 1.00 31.75 ATOM 4860 CB VAL 631 63.649 -3.999 10.007 1.00 24.59	ATOM	4821	N	ARG	627	55.208	3.744	13.378	1.00 23.80
ATOM 4825 CG ARG 627 54.991 6.692 13.055 1.00 27.60 ATOM 4826 CD ARG 627 54.711 8.130 12.584 1.00 33.01 ATOM 4827 NE ARG 627 54.260 8.978 13.691 1.00 34.18 ATOM 4829 CZ ARG 627 52.997 9.067 14.091 1.00 35.88 ATOM 4830 NH1 ARG 627 52.056 8.380 13.460 1.00 38.89 ATOM 4833 NH2 ARG 627 52.056 8.380 13.460 1.00 38.89 ATOM 4833 NH2 ARG 627 52.056 8.380 13.460 1.00 29.03 ATOM 4836 C ARG 627 57.439 4.686 12.785 1.00 29.03 ATOM 4837 O ARG 627 57.439 4.686 12.785 1.00 29.03 ATOM 4838 N ASN 628 57.634 4.938 14.087 1.00 29.51 ATOM 4840 CA ASN 628 58.954 5.234 14.645 1.00 26.41 ATOM 4841 CB ASN 628 58.954 5.234 14.645 1.00 26.41 ATOM 4842 CG ASN 628 58.864 5.359 15.676 1.00 25.32 ATOM 4843 OD1 ASN 628 58.539 7.687 15.035 1.00 22.09 ATOM 4844 ND2 ASN 628 58.539 7.687 15.628 1.00 27.88 ATOM 4847 C ASN 628 59.079 8.028 13.999 1.00 32.09 ATOM 4848 N ASN 628 59.684 4.039 15.225 1.00 25.77 ATOM 4848 O ASN 628 59.684 4.039 15.225 1.00 25.77 ATOM 4848 O ASN 628 59.684 4.039 15.225 1.00 25.77 ATOM 4848 O ASN 628 59.684 4.039 15.225 1.00 25.77 ATOM 4848 O ASN 628 628 58.816 1.00 15.315 1.00 22.96 ATOM 4851 CA VAL 629 59.209 2.853 14.874 1.00 26.63 ATOM 4851 CA VAL 629 59.209 2.853 14.874 1.00 26.53 ATOM 4854 CG2 VAL 629 59.828 1.610 15.315 1.00 25.34 ATOM 4854 CG2 VAL 629 59.492 -0.604 16.412 1.00 22.96 ATOM 4854 CG2 VAL 629 59.492 -0.604 16.412 1.00 22.96 ATOM 4855 C VAL 629 59.492 -0.604 16.412 1.00 22.96 ATOM 4856 O VAL 629 59.492 -0.604 16.412 1.00 22.95 ATOM 4856 O VAL 629 59.492 -0.604 16.412 1.00 22.95 ATOM 4856 O VAL 629 59.492 -0.604 16.412 1.00 22.95 ATOM 4856 O VAL 629 59.492 -0.604 16.412 1.00 22.95 ATOM 4856 O VAL 629 59.492 -0.604 16.412 1.00 22.95 ATOM 4856 O VAL 629 59.492 -0.604 16.412 1.00 22.95 ATOM 4856 O VAL 629 59.492 -0.604 16.412 1.00 22.95 ATOM 4856 O VAL 629 60.266 0.962 14.007 1.00 16.55 ATOM 4860 CB LEU 630 62.667 -1.492 12.961 1.00 28.01 ATOM 4860 CB LEU 630 62.667 -1.492 12.961 1.00 28.01 ATOM 4860 CB LEU 630 62.667 -1.492 12.961 1.00 28.01 ATOM 4860 CB LEU 630 62.667 -1.492 12.996 1.00 28.01 ATOM 4860 C	MOTA	4823	CA	ARG	627	55.980	4.413	12.338	1.00 26.57
ATOM	ATOM	4824	CB	ARG	627	55.289	5.728	11.914	1.00 25.91
ATOM	ATOM	4825	CG	ARG	627	54.991	6.692	13.055	1.00 27.60
ATOM	MOTA	4826	CD		627	54.711			
ATOM 4829 CZ ARG 627 52.997 9.067 14.091 1.00 35.88 ATOM 4830 NHI ARG 627 52.056 8.380 13.46c 1.00 38.89 ATOM 4833 NH2 ARG 627 52.689 9.748 15.183 1.00 36.43 ATOM 4836 C ARG 627 57.439 4.686 12.785 1.00 29.03 ATOM 4837 O ARG 627 58.362 4.636 11.972 1.00 29.24 ATOM 4838 N ASN 628 57.634 4.938 14.087 1.00 29.51 ATOM 4840 CA ASN 628 58.954 5.234 14.645 1.00 26.41 ATOM 4841 CB ASN 628 58.864 5.359 15.676 1.00 25.32 ATOM 4842 CG ASN 628 58.539 7.687 15.035 1.00 28.11 ATOM 4843 NDL ASN 628 59.079 8.028 13.999 1.00 27.88 ATOM 4844 NDL ASN 628 59.079 8.028 13.999 1.00 25.77 ATOM 4848 O ASN 628 59.684 4.039 15.225 1.00 25.77 ATOM 4848 O ASN 628 59.684 4.039 15.225 1.00 25.77 ATOM 4848 O ASN 628 59.884 4.039 15.225 1.00 25.77 ATOM 4849 N VAL 629 59.884 4.039 15.225 1.00 24.77 ATOM 4849 N VAL 629 59.884 1.610 15.315 1.00 24.77 ATOM 4851 CA VAL 629 59.828 1.610 15.315 1.00 22.34 ATOM 4851 CA VAL 629 59.828 1.610 15.315 1.00 22.36 ATOM 4855 C VAL 629 58.812 0.693 16.007 1.00 21.26 ATOM 4855 C VAL 629 59.492 -0.604 16.412 1.00 22.96 ATOM 4856 O VAL 629 59.494 0.839 13.997 1.00 26.79 ATOM 4857 N LEU 630 63.544 0.839 13.997 1.00 26.79 ATOM 4856 C VAL 629 59.454 0.839 13.997 1.00 26.95 ATOM 4860 CB LEU 630 63.297 0.733 12.210 1.00 22.79 ATOM 4861 CG LEU 630 63.297 0.733 12.210 1.00 22.79 ATOM 4862 CD LEU 630 63.297 0.733 12.210 1.00 22.79 ATOM 4866 C LEU 630 62.667 -1.492 12.961 1.00 22.79 ATOM 4868 CA VAL 631 62.468 -3.790 12.998 1.00 30.82 ATOM 4868 CA VAL 631 62.468 -3.790 12.998 1.00 30.82 ATOM 4868 CA VAL 631 62.468 -3.790 12.998 1.00 30.04 ATOM 4868 CA VAL 631 62.468 -3.790 12.098 1.00 30.94 ATOM 4868 CA VAL 631 62.468 -3.790 12.098 1.00 30.94 ATOM 4867 CG VAL 631 63.697 -4.286 11.305 1.00 30.94 ATOM 4867 CG VAL 631 63.697 -4.286 11.305 1.00 30.94 ATOM 4870 CGI VAL 631 63.697 -4.286 11.305 1.00 30.04 ATOM 4871 CGI VAL 631 63.697 -4.286 11.305 1.00 30.04 ATOM 4872 C VAL 631 63.697 -4.286 11.305 1.00 35.24 ATOM 4873 O VAL 631 63.697 -4.286 11.305 1.00 35.24	ATOM	4827	NE		627				
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ATOM 4852 CB VAL 629 58.812 0.693 16.007 1.00 21.26 ATOM 4853 CG1 VAL 629 59.492 -0.604 16.412 1.00 22.96 ATOM 4854 CG2 VAL 629 58.205 1.398 17.207 1.00 16.65 ATOM 4855 C VAL 629 60.266 0.962 14.007 1.00 26.79 ATOM 4856 O VAL 629 59.454 0.839 13.087 1.00 28.60 ATOM 4857 N LEU 630 61.542 0.603 13.904 1.00 25.91 ATOM 4859 CA LEU 630 62.062 -0.021 12.685 1.00 26.95 ATOM 4860 CB LEU 630 63.297 0.733 12.210 1.00 22.79 ATOM 4861 CG LEU 630 63.044 2.242 12.111 1.00 20.04 ATOM 4862 CD1 LEU 630 64.345 2.944 11.972 1.00 11.86 ATOM 4863 CD2 LEU 630 62.111 2.603 10.965 1.00 19.22 ATOM 4864 C LEU 630 62.367 -1.492 12.961 1.00 28.01 ATOM 4865 O LEU 630 62.629 -1.852 14.101 1.00 28.01 ATOM 4866 N VAL 631 62.246 -2.346 11.946 1.00 30.82 ATOM 4868 CA VAL 631 62.468 -3.790 12.098 1.00 31.75 ATOM 4869 CB VAL 631 61.194 -4.607 11.659 1.00 30.04 ATOM 4869 CB VAL 631 61.346 -6.085 12.026 1.00 29.25 ATOM 4870 CG1 VAL 631 61.346 -6.085 12.026 1.00 29.25 ATOM 4871 CG2 VAL 631 63.697 -4.286 11.305 1.00 35.24 ATOM 4873 O VAL 631 63.849 -3.999 10.097 1.00 34.02 ATOM 4873 O VAL 631 63.849 -3.999 10.097 1.00 34.02						5.9.209		14.874	1.00 26.63
ATOM 4853 CG1 VAL 629 59.492 -0.604 16.412 1.00 22.96 ATOM 4854 CG2 VAL 629 58.205 1.398 17.207 1.00 16.65 ATOM 4855 C VAL 629 60.266 0.962 14.007 1.00 26.79 ATOM 4856 O VAL 629 59.454 0.839 13.087 1.00 28.60 ATOM 4857 N LEU 630 61.542 0.603 13.904 1.00 25.91 ATOM 4859 CA LEU 630 62.062 -0.021 12.685 1.00 26.95 ATOM 4860 CB LEU 630 63.297 0.733 12.210 1.00 22.79 ATOM 4861 CG LEU 630 63.044 2.242 12.111 1.00 20.04 ATOM 4862 CD1 LEU 630 64.345 2.944 11.972 1.00 11.86 ATOM 4863 CD2 LEU 630 62.367 -1.492 12.961 1.00 28.01 ATOM 4864 C LEU 630 62.367 -1.492 12.961 1.00 28.01 ATOM 4865 O LEU 630 62.629 -1.852 14.101 1.00 28.26 ATOM 4866 N VAL 631 62.246 -2.346 11.946 1.00 30.82 ATOM 4868 CA VAL 631 62.246 -2.346 11.946 1.00 30.82 ATOM 4869 CB VAL 631 62.468 -3.790 12.098 1.00 31.75 ATOM 4869 CB VAL 631 61.194 -4.607 11.659 1.00 30.04 ATOM 4870 CG1 VAL 631 61.346 -6.085 12.026 1.00 29.25 ATOM 4871 CG2 VAL 631 59.937 -4.030 12.290 1.00 24.59 ATOM 4873 O VAL 631 63.697 -4.286 11.305 1.00 35.24 ATOM 4873 O VAL 631 63.849 -3.999 10.097 1.00 34.02 ATOM 4873 O VAL 631 63.849 -3.999 10.097 1.00 34.02 ATOM 4873 O VAL 631 63.849 -3.999 10.097 1.00 34.02 ATOM 4874 N THR 632 64.551 -5.052 11.979 1.00 36.24								15.315	1.00 25.34
ATOM 4854 CG2 VAL 629 58.205 1.398 17.207 1.00 16.65  ATOM 4855 C VAL 629 60.266 0.962 14.007 1.00 26.79  ATOM 4856 O VAL 629 59.454 0.839 13.087 1.00 28.60  ATOM 4857 N LEU 630 61.542 0.603 13.904 1.00 25.91  ATOM 4859 CA LEU 630 62.062 -0.021 12.685 1.00 26.95  ATOM 4860 CB LEU 630 63.297 0.733 12.210 1.00 22.79  ATOM 4861 CG LEU 630 63.044 2.242 12.111 1.00 20.04  ATOM 4862 CD1 LEU 630 64.345 2.944 11.972 1.00 11.86  ATOM 4863 CD2 LEU 630 62.111 2.603 10.965 1.00 19.22  ATOM 4864 C LEU 630 62.367 -1.492 12.961 1.00 28.01  ATOM 4865 O LEU 630 62.629 -1.852 14.101 1.00 28.26  ATOM 4866 N VAL 631 62.246 -2.346 11.946 1.00 30.82  ATOM 4869 CB VAL 631 62.468 -3.790 12.098 1.00 31.75  ATOM 4869 CB VAL 631 61.194 -4.607 11.659 1.00 30.04  ATOM 4870 CG1 VAL 631 61.346 -6.085 12.026 1.00 29.25  ATOM 4871 CG2 VAL 631 59.937 -4.030 12.290 1.00 24.59  ATOM 4872 C VAL 631 63.697 -4.286 11.305 1.00 35.24  ATOM 4873 O VAL 631 63.849 -3.999 10.097 1.00 34.02  ATOM 4874 N THR 632 64.551 -5.052 11.979 1.00 36.24								16.007	
ATOM 4855 C VAL 629 60.266 0.962 14.007 1.00 26.79 ATOM 4856 O VAL 629 59.454 0.839 13.087 1.00 28.60 ATOM 4857 N LEU 630 61.542 0.603 13.904 1.00 25.91 ATOM 4859 CA LEU 630 62.062 -0.021 12.685 1.00 26.95 ATOM 4860 CB LEU 630 63.297 0.733 12.210 1.00 22.79 ATOM 4861 CG LEU 630 63.044 2.242 12.111 1.00 20.04 ATOM 4862 CD1 LEU 630 64.345 2.944 11.972 1.00 11.86 ATOM 4863 CD2 LEU 630 62.111 2.603 10.965 1.00 19.22 ATOM 4864 C LEU 630 62.367 -1.492 12.961 1.00 28.01 ATOM 4865 O LEU 630 62.629 -1.852 14.101 1.00 28.26 ATOM 4866 N VAL 631 62.246 -2.346 11.946 1.00 30.82 ATOM 4868 CA VAL 631 62.246 -2.346 11.946 1.00 30.82 ATOM 4869 CB VAL 631 61.194 -4.607 11.659 1.00 30.04 ATOM 4870 CG1 VAL 631 61.194 -4.607 11.659 1.00 30.04 ATOM 4871 CG2 VAL 631 59.937 -4.030 12.290 1.00 24.59 ATOM 4873 O VAL 631 63.849 -3.999 10.097 1.00 34.02 ATOM 4873 O VAL 631 63.849 -3.999 10.097 1.00 34.02 ATOM 4873 N THR 632 64.551 -5.052 11.979 1.00 36.24						59.492	-0.604	16.412	1.00 22.96
ATOM 4856 O VAL 629 59.454 0.839 13.087 1.00 28.60 ATOM 4857 N LEU 630 61.542 0.603 13.904 1.00 25.91 ATOM 4859 CA LEU 630 62.062 -0.021 12.685 1.00 26.95 ATOM 4860 CB LEU 630 63.297 0.733 12.210 1.00 22.79 ATOM 4861 CG LEU 630 63.044 2.242 12.111 1.00 20.04 ATOM 4862 CD1 LEU 630 64.345 2.944 11.972 1.00 11.86 ATOM 4863 CD2 LEU 630 62.111 2.603 10.965 1.00 19.22 ATOM 4864 C LEU 630 62.367 -1.492 12.961 1.00 28.01 ATOM 4865 O LEU 630 62.629 -1.852 14.101 1.00 28.26 ATOM 4866 N VAL 631 62.246 -2.346 11.946 1.00 30.82 ATOM 4868 CA VAL 631 62.246 -2.346 11.946 1.00 30.82 ATOM 4869 CB VAL 631 62.468 -3.790 12.098 1.00 31.75 ATOM 4870 CG1 VAL 631 61.194 -4.607 11.659 1.00 30.04 ATOM 4870 CG1 VAL 631 61.346 -6.085 12.026 1.00 29.25 ATOM 4871 CG2 VAL 631 59.937 -4.030 12.290 1.00 24.59 ATOM 4873 O VAL 631 63.849 -3.999 10.097 1.00 34.02 ATOM 4873 O VAL 631 63.849 -3.999 10.097 1.00 34.02 ATOM 4874 N THR 632 64.551 -5.052 11.979 1.00 36.24	ATOM	4854		VAL	629	. 58.205	1.398	17.207	1.00 16.65
ATOM 4857 N LEU 630 61.542 0.603 13.904 1.00 25.91 ATOM 4859 CA LEU 630 62.062 -0.021 12.685 1.00 26.95 ATOM 4860 CB LEU 630 63.297 0.733 12.210 1.00 22.79 ATOM 4861 CG LEU 630 63.044 2.242 12.111 1.00 20.04 ATOM 4862 CD1 LEU 630 64.345 2.944 11.972 1.00 11.86 ATOM 4863 CD2 LEU 630 62.111 2.603 10.965 1.00 19.22 ATOM 4864 C LEU 630 62.367 -1.492 12.961 1.00 28.01 ATOM 4865 O LEU 630 62.629 -1.852 14.101 1.00 28.26 ATOM 4866 N VAL 631 62.246 -2.346 11.946 1.00 30.82 ATOM 4868 CA VAL 631 62.468 -3.790 12.098 1.00 31.75 ATOM 4869 CB VAL 631 61.194 -4.607 11.659 1.00 30.04 ATOM 4870 CG1 VAL 631 61.194 -4.607 11.659 1.00 30.04 ATOM 4871 CG2 VAL 631 59.937 -4.030 12.290 1.00 24.59 ATOM 4872 C VAL 631 63.697 -4.286 11.305 1.00 35.24 ATOM 4873 O VAL 631 63.849 -3.999 10.097 1.00 34.02 ATOM 4874 N THR 632 64.551 -5.052 11.979 1.00 36.24	MOTA	4855	C	VAL	629	60.266	0.962	14.007	1.00 26.79
ATOM 4859 CA LEU 630 62.062 -0.021 12.685 1.00 26.95 ATOM 4860 CB LEU 630 63.297 0.733 12.210 1.00 22.79 ATOM 4861 CG LEU 630 63.044 2.242 12.111 1.00 20.04 ATOM 4862 CD1 LEU 630 64.345 2.944 11.972 1.00 11.86 ATOM 4863 CD2 LEU 630 62.111 2.603 10.965 1.00 19.22 ATOM 4864 C LEU 630 62.367 -1.492 12.961 1.00 28.01 ATOM 4865 O LEU 630 62.629 -1.852 14.101 1.00 28.26 ATOM 4866 N VAL 631 62.246 -2.346 11.946 1.00 30.82 ATOM 4868 CA VAL 631 62.246 -3.790 12.098 1.00 31.75 ATOM 4869 CB VAL 631 61.194 -4.607 11.659 1.00 30.04 ATOM 4870 CG1 VAL 631 61.346 -6.085 12.026 1.00 29.25 ATOM 4871 CG2 VAL 631 59.937 -4.030 12.290 1.00 24.59 ATOM 4872 C VAL 631 63.697 -4.286 11.305 1.00 35.24 ATOM 4873 O VAL 631 63.849 -3.999 10.097 1.00 34.02 ATOM 4874 N THR 632 64.551 -5.052 11.979 1.00 36.24	MOTA	4856	0	VAL	629	59.454	0.839	13.087	1.00 28.60
ATOM 4860 CB LEU 630 63.297 0.733 12.210 1.00 22.79 ATOM 4861 CG LEU 630 63.044 2.242 12.111 1.00 20.04 ATOM 4862 CD1 LEU 630 64.345 2.944 11.972 1.00 11.86 ATOM 4863 CD2 LEU 630 62.111 2.603 10.965 1.00 19.22 ATOM 4864 C LEU 630 62.367 -1.492 12.961 1.00 28.01 ATOM 4865 O LEU 630 62.629 -1.852 14.101 1.00 28.26 ATOM 4866 N VAL 631 62.246 -2.346 11.946 1.00 30.82 ATOM 4868 CA VAL 631 62.468 -3.790 12.098 1.00 31.75 ATOM 4869 CB VAL 631 61.194 -4.607 11.659 1.00 30.04 ATOM 4870 CG1 VAL 631 61.346 -6.085 12.026 1.00 29.25 ATOM 4871 CG2 VAL 631 59.937 -4.030 12.290 1.00 24.59 ATOM 4872 C VAL 631 63.697 -4.286 11.305 1.00 35.24 ATOM 4873 O VAL 631 63.849 -3.999 10.097 1.00 34.02 ATOM 4874 N THR 632 64.551 -5.052 11.979 1.00 36.24	MOTA	4857	N	LEU	630	61.542	0.603	13.904	1.00 25.91
ATOM 4861 CG LEU 630 63.044 2.242 12.111 1.00 20.04 ATOM 4862 CD1 LEU 630 64.345 2.944 11.972 1.00 11.86 ATOM 4863 CD2 LEU 630 62.111 2.603 10.965 1.00 19.22 ATOM 4864 C LEU 630 62.367 -1.492 12.961 1.00 28.01 ATOM 4865 O LEU 630 62.629 -1.852 14.101 1.00 28.26 ATOM 4866 N VAL 631 62.246 -2.346 11.946 1.00 30.82 ATOM 4868 CA VAL 631 62.468 -3.790 12.098 1.00 31.75 ATOM 4869 CB VAL 631 61.194 -4.607 11.659 1.00 30.04 ATOM 4870 CG1 VAL 631 61.346 -6.085 12.026 1.00 29.25 ATOM 4871 CG2 VAL 631 59.937 -4.030 12.290 1.00 24.59 ATOM 4873 O VAL 631 63.697 -4.286 11.305 1.00 35.24 ATOM 4873 O VAL 631 63.849 -3.999 10.097 1.00 34.02 ATOM 4874 N THR 632 64.551 -5.052 11.979 1.00 36.24	ATOM	4859	CA	LEU	630	62.062	-0.021	12.685	1.00 26.95
ATOM 4862 CD1 LEU 630 64.345 2.944 11.972 1.00 11.86 ATOM 4863 CD2 LEU 630 62.111 2.603 10.965 1.00 19.22 ATOM 4864 C LEU 630 62.367 -1.492 12.961 1.00 28.01 ATOM 4865 O LEU 630 62.629 -1.852 14.101 1.00 28.26 ATOM 4866 N VAL 631 62.246 -2.346 11.946 1.00 30.82 ATOM 4868 CA VAL 631 62.468 -3.790 12.098 1.00 31.75 ATOM 4869 CB VAL 631 61.194 -4.607 11.659 1.00 30.04 ATOM 4870 CG1 VAL 631 61.346 -6.085 12.026 1.00 29.25 ATOM 4871 CG2 VAL 631 59.937 -4.030 12.290 1.00 24.59 ATOM 4872 C VAL 631 63.697 -4.286 11.305 1.00 35.24 ATOM 4873 O VAL 631 63.849 -3.999 10.097 1.00 34.02 ATOM 4874 N THR 632 64.551 -5.052 11.979 1.00 36.24	MOTA	4860	CB	LEU	630	63.297	0.733	12.210	1.00 22.79
ATOM 4863 CD2 LEU 630 62.111 2.603 10.965 1.00 19.22 ATOM 4864 C LEU 630 62.367 -1.492 12.961 1.00 28.01 ATOM 4865 O LEU 630 62.629 -1.852 14.101 1.00 28.26 ATOM 4866 N VAL 631 62.246 -2.346 11.946 1.00 30.82 ATOM 4868 CA VAL 631 62.468 -3.790 12.098 1.00 31.75 ATOM 4869 CB VAL 631 61.194 -4.607 11.659 1.00 30.04 ATOM 4870 CG1 VAL 631 61.346 -6.085 12.026 1.00 29.25 ATOM 4871 CG2 VAL 631 59.937 -4.030 12.290 1.00 24.59 ATOM 4872 C VAL 631 63.697 -4.286 11.305 1.00 35.24 ATOM 4873 O VAL 631 63.849 -3.999 10.097 1.00 34.02 ATOM 4874 N THR 632 64.551 -5.052 11.979 1.00 36.24	ATOM	4861	CG	LEU	630	63.044	2.242	12.111	1.00 20.04
ATOM 4863 CD2 LEU 630 62.111 2.603 10.965 1.00 19.22  ATOM 4864 C LEU 630 62.367 -1.492 12.961 1.00 28.01  ATOM 4865 O LEU 630 62.629 -1.852 14.101 1.00 28.26  ATOM 4866 N VAL 631 62.246 -2.346 11.946 1.00 30.82  ATOM 4868 CA VAL 631 62.468 -3.790 12.098 1.00 31.75  ATOM 4869 CB VAL 631 61.194 -4.607 11.659 1.00 30.04  ATOM 4870 CG1 VAL 631 61.346 -6.085 12.026 1.00 29.25  ATOM 4871 CG2 VAL 631 59.937 -4.030 12.290 1.00 24.59  ATOM 4872 C VAL 631 63.697 -4.286 11.305 1.00 35.24  ATOM 4873 O VAL 631 63.849 -3.999 10.097 1.00 34.02  ATOM 4874 N THR 632 64.551 -5.052 11.979 1.00 36.24	ATOM	4862	CD1	LEU	630	64.345	2.944	11.972	1.00 11.86
ATOM 4864 C LEU 630 62.367 -1.492 12.961 1.00 28.01 ATOM 4865 O LEU 630 62.629 -1.852 14.101 1.00 28.26 ATOM 4866 N VAL 631 62.246 -2.346 11.946 1.00 30.82 ATOM 4868 CA VAL 631 62.468 -3.790 12.098 1.00 31.75 ATOM 4869 CB VAL 631 61.194 -4.607 11.659 1.00 30.04 ATOM 4870 CG1 VAL 631 61.346 -6.085 12.026 1.00 29.25 ATOM 4871 CG2 VAL 631 59.937 -4.030 12.290 1.00 24.59 ATOM 4872 C VAL 631 63.697 -4.286 11.305 1.00 35.24 ATOM 4873 O VAL 631 63.849 -3.999 10.097 1.00 34.02 ATOM 4874 N THR 632 64.551 -5.052 11.979 1.00 36.24	ATOM	4863	CD2	LEU	630	62.111			
ATOM 4865 O LEU 630 62.629 -1.852 14.101 1.00 28.26 ATOM 4866 N VAL 631 62.246 -2.346 11.946 1.00 30.82 ATOM 4868 CA VAL 631 62.468 -3.790 12.098 1.00 31.75 ATOM 4869 CB VAL 631 61.194 -4.607 11.659 1.00 30.04 ATOM 4870 CG1 VAL 631 61.346 -6.085 12.026 1.00 29.25 ATOM 4871 CG2 VAL 631 59.937 -4.030 12.290 1.00 24.59 ATOM 4872 C VAL 631 63.697 -4.286 11.305 1.00 35.24 ATOM 4873 O VAL 631 63.849 -3.999 10.097 1.00 34.02 ATOM 4874 N THR 632 64.551 -5.052 11.979 1.00 36.24	ATOM	4864	С	LEU		62.367			
ATOM 4866 N VAL 631 62.246 -2.346 11.946 1.00 30.82  ATOM 4868 CA VAL 631 62.468 -3.790 12.098 1.00 31.75  ATOM 4869 CB VAL 631 61.194 -4.607 11.659 1.00 30.04  ATOM 4870 CG1 VAL 631 61.346 -6.085 12.026 1.00 29.25  ATOM 4871 CG2 VAL 631 59.937 -4.030 12.290 1.00 24.59  ATOM 4872 C VAL 631 63.697 -4.286 11.305 1.00 35.24  ATOM 4873 O VAL 631 63.849 -3.999 10.097 1.00 34.02  ATOM 4874 N THR 632 64.551 -5.052 11.979 1.00 36.24	ATOM								
ATOM 4868 CA VAL 631 62.468 -3.790 12.098 1.00 31.75 ATOM 4869 CB VAL 631 61.194 -4.607 11.659 1.00 30.04 ATOM 4870 CG1 VAL 631 61.346 -6.085 12.026 1.00 29.25 ATOM 4871 CG2 VAL 631 59.937 -4.030 12.290 1.00 24.59 ATOM 4872 C VAL 631 63.697 -4.286 11.305 1.00 35.24 ATOM 4873 O VAL 631 63.849 -3.999 10.097 1.00 34.02 ATOM 4874 N THR 632 64.551 -5.052 11.979 1.00 36.24									
ATOM 4869 CB VAL 631 61.194 -4.607 11.659 1.00 30.04 ATOM 4870 CG1 VAL 631 61.346 -6.085 12.026 1.00 29.25 ATOM 4871 CG2 VAL 631 59.937 -4.030 12.290 1.00 24.59 ATOM 4872 C VAL 631 63.697 -4.286 11.305 1.00 35.24 ATOM 4873 O VAL 631 63.849 -3.999 10.097 1.00 34.02 ATOM 4874 N THR 632 64.551 -5.052 11.979 1.00 36.24									
ATOM 4870 CG1 VAL 631 61.346 -6.085 12.026 1.00 29.25 ATOM 4871 CG2 VAL 631 59.937 -4.030 12.290 1.00 24.59 ATOM 4872 C VAL 631 63.697 -4.286 11.305 1.00 35.24 ATOM 4873 O VAL 631 63.849 -3.999 10.097 1.00 34.02 ATOM 4874 N THR 632 64.551 -5.052 11.979 1.00 36.24									
ATOM 4871 CG2 VAL 631 59.937 -4.030 12.290 1.00 24.59 ATOM 4872 C VAL 631 63.697 -4.286 11.305 1.00 35.24 ATOM 4873 O VAL 631 63.849 -3.999 10.097 1.00 34.02 ATOM 4874 N THR 632 64.551 -5.052 11.979 1.00 36.24									
ATOM 4872 C VAL 631 63.697 -4.286 11.305 1.00 35.24 ATOM 4873 O VAL 631 63.849 -3.999 10.097 1.00 34.02 ATOM 4874 N THR 632 64.551 -5.052 11.979 1.00 36.24									
ATOM 4873 O VAL 631 63.849 -3.999 10.097 1.00 34.02 ATOM 4874 N THR 632 64.551 -5.052 11.979 1.00 36.24									
ATOM 4874 N THR 632 64.551 -5.052 11.979 1.00 36.24									
ATOM 4876 CA THR 632 65.770 -5.574 11.365 1.00 38.23									
	ATOM	4876	CA	THR	632	65.770	-5.574	11.365	1.00 38.23





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ATOM	4941	С	LYS	638	63.443	0.364	17.446	1.00 28.00
ATOM	4942	0	LYS	638	62.977	0.799	16.391	1.00 25.60
ATOM	4943	N	ILE	639	63.410	1.032	18.601	1.00 25.32
ATOM	4945	CA	ILE	639	62.857	2.379	18.721	1.00 25.91
MOTA	4946	CB	ILE	639	62.800	2.875	20.201	1.00 25.56
MOTA	4947	CG2	ILE	639	62.074	4.208	20.279	1.00 22.82
ATOM	4948	CG1	ILE	639	62.142	1.835	21.118	1.00 28.00
MOTA	4949	CD1	ILE	639	60.634	1.748	21.003	1.00 33.25
ATOM	4950	С	ILE	639	63.739	3.363	17.955	1.00 26.87
MOTA	4951	0	ILE	639	64.968	3.381	18.125	1.00 24.13
MOTA	4952	N	ALA	640	63.108	4.170	17.108	1.00 26.74
ATOM	4954	CA	ALA	640	63.825	5.176	16.339	1.00 30.62
ATOM	4955	CB	ALA	640	63.624	4.939	14.851	1.00 30.31
MOTA	4956	C	ALA	640	63.338	6.572	16.739	1.00 32.53
MOTA	4957	0	ALA	640	62.289	6.706	17.371	1.00 33.83
ATOM	4958	N	ASP	641	64.082	7.605	16.351	1.00 33.05
MOTA	4960	CA	ASP	641	63.749	9.010	16.656	1.00 37.66
MOTA	4961	CB	ASP	641	62.539	9.489	15.840	1.00 42.62
ATOM	4962	CG	ASP	641	62.928	10.026	14.471	1.00 50.92
ATOM	4963		ASP	641	64.092	9.833	14.021	1.00 59.21
ATOM	4964	OD2	ASP	641	62.063	10.652	13.823	1.00 54.05
MOTA	4965	С	ASP	641	63.545	9.367	18.125	1.00 37.85
ATOM	4966	0	ASP	641	62.805	10.294	18.448	1.00 39.10
ATOM	4967	N	PHE	642	64.204	8.635	15.016	1.00 37.47
ATOM	4969	CA	PHE	642	64.099	8.874	20.456	1.00 36.47
MOTA	4970	CB	PHE	642	64.403	7.581	21.226	1.00 32.22
ATOM	4971	CG	PHE	642	65.786	7.013	20.964	1.00 30.65
ATOM	4972	CD1	PHE	642	66 906	7.537	21.607	1.00 32.45
MOTA	4973	CD2	PHE	642	65.969	5.981	20.054	1.00 28.53
MOTA	4974	CE1	PHE	642	68.180	7.050	21.342	1.00 30.88
ATOM	4975	CE2	PHE	642	67.234	5.494	19.789	1.00 27.74
MOTA	4976	CZ	PHE	642	68.344	6.027	20.431	1.00 29.64
MOTA	4977	C	PHE	642	<b>6</b> 5.050	10.001	20.907	1.00 39.69
MOTA	4978	0	PHE	642	64.967	10.469	22.047	1.00 38.22
MOTA	4979	N	GLY	643	65.966	10.400	20.015	1.00 41.08
MOTA	4981	CA	GLY	643	66.925	11.447	20.324	1.00 40.65
ATOM	4982	C	GLY	643	66.694	12.747	19.571	1.00 43.53
ATOM	4983	O	GLY	643	67.500	13.666	19.688	1.00 41.10
ATOM	4984	N	LEU	644	65.617	12.825	18.786	1.00 48.35
MOTA	4986	CA	LEU	644	65.306	14.034	18.019	1.00 51.11
MOTA	4987	CB	LEU	644	63.962	13.907	17.314	1.00 50.28
ATOM	4988	CG	LEU	644	63.900	13.059	16.057	1.00 54.03
ATOM	4989		LEU	644	62.541	13.278	15.413	1.00 57.34
ATOM	4990	CD2	LEU	644	65.006	13.467	15.105	1.00 56.95
MOTA	4991	C	LEU	644	65.248	15.257	18.894	1.00 52.68
ATOM	4992	0	LEU	644	64.850	15.175	20.053	1.00 54.95
ATOM	4993	N	ALA	645	65629	16.399	18.332	1.00 54.61
ATOM	4995	CA	ALA	645	65.610	17.656	19.073	1.00 54.60
MOTA	4996	CB	ALA	645	66.495	18.684	18.382	1.00 53.32
ATOM	4997	С	ALA	645	64.178	18.185	19.215	1.00 54.09
ATOM	4998	0	ALA	645	63.716	18.488	20.322	1.00 53.14
ATOM	4999	N	ASP	652	52.340	21.795	14.895	1.00 91.33

	ሽ ም <b>ር</b> አፋ					
	ATOM	500		ASP	652	2
	ATOM	500	2 CB	ASP	652	21.914 14.004 1 00 00 00
	MOTA	500	3 CG	ASP	652	31.650 22.138 12 555
	MOTA	5004	0D1	ASP		30.488 22.434 11 606
24	MOT	5005	5 OD2	ASP	652	49.479 23.032 12.042
	TOM	5006		ASP	652	50.586 22.075 30.414
A	TOM	5007		•	652	50,352 20 652 40.414 1.00 94.81
		5008		<b>~~</b>	652	50.645 19.643 1.00 90.61
		5010			653	49.289 20.737 13.463 1.00 91.26
			4		653	49 303 30 14.895 1.00 89 65
		5011		TYR (	553	47 306 25 15.110 1.00 88 25
		5012	CG	TYR 6	553	47 000 - 16.133 1.00 88 16
		013	CD1	733.000	553	27.800 20.140 17.559 1 00 00 7
	OM 5	014			53	20.818 18.513 1 00 00
	OM 5	015			53	3/.4// 20.915 19.910
AT		016		***		49.006 19.559 17.964
AT		017			53	49.443 19.649 19.300 "
AT		018	_		53	48.675 20 225 - 3.00 89.49
ATO	~	020			53	49.109 20.30
ATO	38.0	021	-		53	47.701 19 165 47 1.00 89.81
ATO		22		YR 65	53	47.180 18.053 13.830 1.00 87.32
ATO		24		YR 65	54	47 734 20 1 13 759 1 00 87 76
ATO				/R 65	4	47 007 10 12.814 1.00 86 51
ATO		25	CB T		4	46 302 11.353 1.00 87 00
ATO			CG TY	R 65	4	11.028 1 00 00
	-		CD1 TY	'R 65		15.3/5 21.497 12.014 1.00 00 ==
ATO			CE1 TY	R 65		13.781 22.017 13.246 1 20 20
ATO		29	CD2 TY			22.431 14.197 1.00 00
ATON		30 (	CE2 TY			21.419 11 757
ATOM		31 (	Z TY	-2-3		43.078 21.833 12.600
ATOM		2 (	H TY			43.506 22.335 13.010
ATOM						42.588 22.717 14 972
ATOM	503					48.C12 10 13 - 1.00 94.38
ATOM	503					47.567 18 767
ATOM		_				49.290 18 971 410 1.00 88.29
ATOM	503	_				50.233 18 406 1.00 86.67
ATOM		_		655		51 606 35 9.887 1.00 87 62
ATOM	504(	. •		655		52 699 45 10.229 1.00 90 01
ATOM	504]		LYS	655		54 106 10 95.23
ATOM	5042		LYS	655		9.607 1.00 00 00
	5043		LYS	655		- 8.789 1 00100 -
ATOM	5047		LYS	655		38.528 18.184 9.099 1.00704
ATOM	5048		LYS	655		30.102 16.890 9.896 3 00 07
ATOM	5049	N	LYS	656		30.233 16.259 10.945 1 00 00
ATOM	5051	CA				49.787 16.319 9 777
ATOM	5052	СВ	LYS	656		49.639 14.875 8.603
ATOM	5053	CG		656		48.795 14 523 1.00 89.03
ATOM	5054		LYS	656		47.313 14 803 7.376 1.00 90.44
ATOM	5055	CD	LYS	656		46.590 14 500 7.535 1.00 93.30
ATOM	5056	CE	LYS	656		45.089 14.555 6.213 1.00 96.87
ATOM		NZ	LYS	656		44 363 44 363 4.406 1.00 99 35
ATOM	5060	C	LYS	656		51 004 5.106 1.00102 42
	5061	0	LYS	656		31.004 14.206 8.487 1.00.00 ==
ATOM	5062	N	GLY	660		7.855 1 00 00 00
ATOM	5064	CA	GLY	660		19.270 10.021 5.735 1.00 6
ATOM	5065	С	GLY	660	•	48.416 11.168 6.005 3.00 50 77
				500	4	47.664 21.000
C00-						7.324 1.00 57.22
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MOTA	5066	0	GLY	660	46.555	11.624	7.437	1.00 58.01
ATOM	5067	N	ARG	661	48.231	10.374	8.293	1.00 55.37
ATOM	5069	CA	ARG	661	47.631	10.247	9.622	1.00 51.19
ATOM	5070	CB	ARG	661	48.095	8.965	10.337	1.00 51.89
MOTA	5071	CG	ARG	661	47.756	7.663	9.612	1.00 51.56
MOTA	5072	CD	ARG	661	48.057	6.443	10.484	1.00 50.77
MOTA	5073	NE	ARG	661	47.834	5.181	9.772	1.00 50.04
ATOM	5075	CZ	ARG	661	48.015	3.974	10.307	1.00 48.12
ATOM	5076	NH1	ARG	661	48.421	3.855	11.569	1.00 43.28
ATOM	5079	NH2		661	47.788	2.882	9.578	1.00 43.69
ATOM	5082	С	AR.G	661	48.041	11.463	10.446	1.00 46.22
ATOM	5083	0	ARG	661	48.998	12.162	10.097	1.00 44.78
ATOM	5084	N	LEU	662	47.328	11.703	11.542	1.00 41.80
MOTA	5086	CA	LEU	662	47.621	12.837	12.419	1.00 36.78
MOTA	5087	CB	LEU	662	46.342	13.596	12.758	1.00 33.05
ATOM	5088	ĊĠ	LEU	662	45.642	14.279	11.585	1.00 28.24
ATOM	5089		LEU	662	44.198	14.611	11.935	1.00 24.66
MOTA	5090	CD2	LEU	662	46.429	15.511	11.217	1.00 28.35
ATOM	5091	C	LEU	662	48.278	12.328	13.695	1.00 36.10
MOTA	5092	C	LEU	662	47.695	11.521	14.431	1.00 34.46
MOTA	5093	N	PRO	663	49.526	12.751	13.945	1.00 35.83
MOTA	5094	CD	PRO	663	50.360	13.537	13.022	1.00 37.72
MOTA	5095	CA	PRO	663	50.310	12.365	15.119	1.00 35.68
ATOM	5096	C.B	PRO	663	51.611	13.130	14.914	1.00 35.23
ATOM	5097	CG	PRO	563	51.756	13.134	13.437	1.00 36.10
MOTA	5098	C	PRO	663	49.660 .	12 703	16.453	1.00 35.87
ATOM	5099	0	PRO	663	49.958	12.069	17.469	1.00 39.86
ATOM	5100	N	VAL	664	48.787	13, 705	16.466	1.00 33.54
ATOM	5102	CA	VAL	664	48.109	14.076	17.699	1.00 31.24
ATOM	5103	CB	VAL	664	47.196	15.321	17.520	1.00 30.45
ATOM	5104	CG1		664	48.025	16.480	17.051	1.00 32.54
MOTA	5105	CG2		664	46.093	15.062	16.523	1.00 34.77
ATOM	5106	C	VAL	664	47.301	12.895	18.233	1.00 31.33
ATOM	5107	0	VAL	664	47.095	12.782	19.438	1.00 32.66
MOTA	5108	N	LYS	665	46.940	11.968	17.345	1.00 30.44
ATOM	5110	CA	LYS	665	46.153	10.795	17.719	1.00 28.43
ATOM	5111	CB	LYS	665	45.596	10.133	16.466	1.00 24.82
ATOM	5112	CG	LYS	665	44.700	11.080	15.687	1.00 27.50
ATOM	5113	CD	LYS	665	44.096	10.466	14.442	1.00 26.62
ATOM	5114	CE	LYS	665	42.967	11.326	13.909	1.00 21.64
ATOM	5115	NZ	LYS	665	42.479	10.850	12.584	1.00 25.29
ATOM	5119	C	LYS	665	46.889	9.794	18.615	1.00 29.56
ATOM	5120	0	LYS	665	46.295	8.836	19.095	1.00 29.57
ATOM	5121	N	TRP	666	48.183	10.020	18.826	1.00 30.12
ATOM	5123	CA	TRP	666	48.987	9.174	19.704	1.00 31.39
MOTA	5124	CB	TRP	666	50.329	8.845	19.059	1.00 30.40
MOTA	5125	CG	TRP	666	50.263	7.700	18.106	1.00 30.79
MOTA	5126		TRP	666	49.701	7.719	16.785	1.00 30.22
MOTA	5127		TRP	666	49.891	6.430	16.245	1.00 28.24
MOTA	5128	CE3		666	49.067	8.702	16.012	1.00 30.60
ATOM	5129	CD1		666	50.743	6.435	18.307	1.00 28.07
ATOM	5130	NE1	TRP	666	50.522	5.670	17.187	1.00 29.15

יית	гом	F 7 7 ^	_		
		5132	CZ2		
		5133	_	TRP 666	48.640 9 224 1.00 29.38
		5134		TRP 666	48.845 7.005
AT	^	5135	_	TRP 666	49 242 0 000 14.213 1.00 31.33
AT		3136		RP 666	49.591 0 207 - 1.00 33.92
AT		137		ET 667	49.028 11.214 22.040 1.00 35.23
ATO		139		ET 667	49 260 11.214 21.007 1.00 35 72
ATO	_	140		ET 667	40 163 12.065 22.159 1.00 36.43
	_	141		ET 667	50 510 13.329 21.751 1.00 37.70
ATC	•	142	SD M	ET 667	50 350 21.574 1.00 40.10
ATC	•	143		ET 667	50.014 21.096 1.00 46 91
ATO		144	C M	ET 667	19.386 1.00 40.40
OTA		145	O ME		47 106 23.378 1.00 38 36
ATO		146	N AI		19 007 11.646 23.273 1.00 39.53
ATO		48	CA AL		19 145 24.542 1.00 39 93
ATO		49	CB AL	A 668	10 351 25.815 1.00 38 48
ATO		50	C AL		23.331 11.537 26.929 1 00 37 63
ATOM		51	C AL	_	17.003 13.038 26.014 1.00 39 40
ATOM			N PR		25.566 1.00 39.40
ATOM		53 (	CD PR		26.731 1 00 42 22
ATOM			CA PRO		45.842 11.827 27.355 1 00 42 77
ATOM			B PRO		26.980 1.00 43 91
ATOM			G PRO		13.698 27.948 1.00 44 40
ATOM		57 C	PRO		44 421 12.279 27.499 1.00 42 50
ATOM	515	8 O			46.476 15.372 27.570 1.00 44.20
ATOM	515	9 N			46.394 16.497 27.075 1 00 45 40
ATOM	516	1 C		•	47.266 15.105 28.607 1 00 43 30
ATOM	516	2 C		670	48.050 16.158 29.244 1.00 42 67
ATOM	516	3 C		670	48./39 15.645 30.504 1 00 42 21
ATOM	516	4 C1		670	49.864 14.646 30.252 1.00 44 78
ATOM	516	5 OI	E1 GLU	670	49.408 13.204 30.290 1 00 43 48
ATOM	516	o o	E2 GLU	670	30.225 12.331 30.639 1 00 41 05
ATOM	516	7 C	GLU	670	48.235 12.931 29.986 1 00 42 15
ATOM	5168	3 0	GLU	670	49.090 16.798 28.333 1.00 43 18
ATOM	5169	N	ALA	671	49.362 17.983 28.444 1.00 41.69
ATOM	5171	CA		671	49.677 16.008 27.440 1.00 44 65
MOTA	5172	CB		671	50.686 16.512 26.513 1.00 44 44
ATOM	5173	C	ALA	671	51.412 15.347 25.841 1 00 40 17
MOTA	5174	0	ALA	671	50.046 17.410 25.465 1 00 46 40
ATOM	5175	N	LEU	672	50.558 18.484 25.148 1 00 45 50
ATOM	5177	CA	LEU	672	46.903 16.970 24.952 1 00 50 30
ATOM	5178	CB	LEU	672	48.163 17.702 23.925 1.00 52.07
ATOM	5179	CG	LEU	672	47.080 16.782 23.335 1 00 54 42
MOTA	5180		LEU	672	46.388 17.103 22.005 1 00 57 12
ATOM	5181	CD2	LEU	672	47.404 17.316 20.912 1 00 57 65
MOTA	5182	С	LEU		45.459 15.951 21.640 1.00 56 14
ATOM	5183	0	LEU	672	47.535 18.964 24 512 3 00 50
ATOM	5184	N	PHE	672	47.683 20.058 23.969 1.00 52.71
MOTA	5186	CA	PHE	673	46.863 18.803 25.645 1.00 52.71
ATOM	5187	CB	PHE	673	46.203 19.911 26 314 1 22 -
ATOM	5188	CG	PHE	673	44.995 19.394 27 104 1 00
ATOM	5189		PHE	673	43.987 18.646 26.259 1.00 52.92
		CDI	FNL	673	43 399 17 455
					26.728 1.00 53.49

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MOTA 5190 CD2 PHE 673 43.624 19.109 24.999 1.00 51.61 ATOM 5191 CE1 PHE 673 42.468 16.779 25.957 1.00 50.49 MOTA 5192 CE2 PHE 673 42.698 24.229 18.420 1.00 50.91 **ATOM** 5193 CZPHE 673 42.118 17.250 24.710 1.00 50.09 **ATOM** 5194 C PHE 673 47.138 20.732 27.220 1.00 56.29 ATOM 5195 0 PHE 673 47.289 21.938 27.026 1.00 58.05 **ATOM** 5196 N ASP 674 47.808 20.076 28.165 1.00 56.38 **ATOM** 5198 CA ASP 48.703 674 20.772 29.104 1.00 56.12 ATOM 5199 CB **ASP** 674 48.644 20.101 30.485 1.00 53.81 MOTA 5200 CG ASP 674 47.299 31.152 20.234 1.00 52.48 ATOM 5201 OD1 ASP 674 46.715 19.188 31.504 1.00 50.25 MOTA 5202 OD2 ASP 674 46.844 21.384 31.337 1.00 51.16 MOTA 5203 С ASP 674 50.182 20.886 28.706 1.00 57.07 **ATOM** 5204 0 ASP 674 51.010 21.273 29.541 1.00 56.00 ATOM 5205 N ARG 675 50.525 20.526 27.468 1.00 57.28 MOTA 5207 CA ARG 675 51.915 20.576 26.995 1.00 55.64 CBATOM 5208 ARG 675 52.. 341 22.020 26.692 1.00 58.95 ATOM 5209 CG ARG 675 51.542 22.678 25.569 1.00 66.91 MOTA 5210 CD ARG 675 52.082 24.066 25.202 1.00 72.90 MOTA 5211 NE ARG 675 53.360 24.019 24.482 1.00 75.10 ATOM 5213 CZARG 675 54.096 25.089 24.181 1.00 73.61 ATOM 5214 NH1 ARG 675 53.687 26.301 24.536 1.00 71.27 ATOM 5217 NH2 ARG 675 55.250 24.943 23.540 1.00 72.12 ATOM 5220 С **ARG** 675 52.853 19.932 28.017 1.00 53.25 MOTA 5221 O ARG 675 53.988 20.366 28.211 1.00 52.13 MOTA 5222 N ILE 676 . 52.359 18.883 28.664 1.00 51.44 MOTA 5224 CA ILE 676 53.108 18.153 29.683 1.00 49.81 MOTA 5225 CB ILE 676 52.241 17.944 30.958 1.00 46.07 MOTA 5226 CG2 ILE 676 52.804 16.844 31.856 1.00 40.98 MOTA 5227 CG1 ILE 676 52.129 19.257 31.721 1.00 43.31 MOTA 5228 CD1 ILE 676 51.324 19.147 32.963 1.00 45.02 MOTA 5229  $\mathbf{C}$ ILE 676 53.572 16.800 29.144 1.00 51.20 **ATOM** 5230 0 ILE 52.770 676 15.892 28.951 1.00 52.37 **ATOM** 5231 N TYR 677 54.865 16.675 28.890 1.00 52.81 ATOM 5233 CA TYR 677 55.412 15.429 28.383 1.00 53.96 MOTA 15.700 5234 CB TYR 677 56.296 27.167 1.00 57.26 **ATOM** 5235 CG TYR 677 55.524 16.175 25.951 1.00 64.10 MOTA 5236 CD1 TYR 677 55.229 17.532 25.762 1.00 65.60 MOTA 5237 CE1 TYR 677 54.514 17.965 1.00 67.15 24.634 MOTA 5238 CD2 TYR 677 55.085 15.263 24.985 1.00 66.29 MOTA 5239 CE2 TYR 677 54.376 15.680 23.862 1.00 67.34 MOTA 5240 CZTYR 677 54.095 17.028 23.692 1.00 69.24 ATOM 5241 ОН TYR 677 53.399 17.414 22.573 1.00 73.55 ATOM 5243 C TYR 677 56.192 14.713 29.482 1.00 52.30 ATOM 5244 0 TYR 677 57.053 15.309 30.124 1.00 53.73 **ATOM** 5245 N THR 678 55.830 13.461 29.748 1.00 48.95 MOTA 5247 CA THR 678 56.505 12.659 30.760 1.00 45.99 ATOM 5248 CB THR 678 55.729 12.634 32.107 1.00 46.04 **ATOM** 5249 OG1 THR 678 54.663 11.676 32.046 1.00 49.79

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5251

5252

5253

CG2 THR

THR

THR

C

0

678

678

678

55.160

56.656

56.231

14.010

11.221

10.888

32.429

30.261

29.158

1.00 45.58

1.00 43.81

1.00 45.12

ATOM

**ATOM** 

ATOM

;	ATOM -			
	7 770 -	54 N	HIS 6	79 57 250
	ATOM 52		_	37.250 10.359 31 0-
	ATOM 52	57 CB	**	57.414 8.971 20 575 1.00 41.50
	ATOM 525	58 CG		58.390 8 252 2-100 38.39
	TOM 525	_	*** ~	79 59.798 8 770 33 1.00 38.62
A	TOM 526			60 456 31.524 1.00 41 51
A'	TOM 526		HIS 67	9 60 715 32.2/3 1.00 40 13
A:	TOM 526		HIS 67	9 61 880 30.613 1.00 47 78
	TOM 526	_	HIS 67	9 61 747 30.806 1.00 39 44
	- 220		HIS 67	$9   \frac{9.742}{56.06}   31.807   1.00   43.55$
	520		HIS 679	9 55 222 8.279 30.720 1 00 22 5
			GLN 680	7.215 30.137 1 00 4
AT	O		GLN 680	
711		CB	GLN 680	53.773 8.290 27 42 4.00 39.84
ATO			25	53.021 8.705 32 3.00 38.92
ATO			77	53.518 8.005 34.00 38.21
ATO	DM 5273			53.651 6 477 22 1.00 42.17
ATO	DM 5274			52.686 5 727 33.878 1.00 43.35
ATO	M 5277			54 860 34.056 1.00 44 05
ATO	M 5278		LN 680	53 012 33.564 1.00 37 17
ATO			LN 680	52 220 7 30.221 1.00 39 32
ATO	M 5281		ER 681	53 290 23.709 1.00 40 26
ATON	3201		ER 681	53 9.854 29.673 1.00 20
ATOM	-202		ER 681	52 036 10.251 28.441 1.00 75
ATOM	-200	OG SI	ER 681	71.698 28.078 1 00 17
ATOM		C SE		
		O SE		53.095 9 278 82 2.00 38.03
AT'OM	., 2.0 /	N AS		52.302 R 955 7.00 38.28
ATOM	~203	CA AS	502	54.362 8 966 1.00 39.41
ATOM	5290	CB AS	~ ~ ~ ~ ~ ~ ~ ~ ~ ~ ~ ~ ~ ~ ~ ~ ~ ~ ~	54.920 7 883 1.00 36.81
ATOM		CG AS		56.404 7 655 55 1.00 36.41
MOTA	_	OD1 ASI	00 <sub>2</sub>	57.309 8:504 25 1.00 37.18
ATOM		D2 ASI	<del>-</del>	58 520 - 23.968 1.00 40 00
ATOM				56 924 25.959 1.00 11 94
ATOM	E20=			54 100 - 23.352 1.00 30 55
ATOM	F20-		002	54 005 - 26.645 1.00 36 93
ATOM	F200		683	5.818 25.675 1 00 20 7
ATOM	F00-	A VAL	683	6.268 27.866 7.00 36
ATOM	5299 c		683	53.03. 5.040 28.143 1.00.36.33
ATOM	5300 C	G1 VAL	683	51 22 4.820 29.683 1 00 25 25
ATOM	5301 C	32 VAL	683	54.500 3.653 29.989 1.00 34.55
ATOM	5302 C	VAL	683	4.546 20 220
	5303 <sub>O</sub>	VAL	683	5.067 57 30
MOTA	5304 N	TRP	684	51.223 4.050 26 242
ATOM	5306 CA			51.027 6 245 27 1.00 32.81
ATOM	5307 CB		684	49.759 6.412 26 62 1.00 34.49
ATOM	5308 CG		684	49.200 7.825 26.602 1.00 36.39
ATOM		2 TRP	684	48.006 8 174 27 1.00 39.30
ATOM		י אנה ה זעה	684	46.651 8 301 26 1.00 41.47
ATOM		TRP	684	45 806 26.384 1.00 42 41
7 moss		TRP	684	46 004 25.247 1.00 41 76
		TRP	684	48 010 2 27.627 1.00 42 06
	5313 NE1	TRP	684	46 310 8.410 24.597 1 00 40 75
	5315 CZ2	TRP	684	8.756 24.175 7 00 43 33
	5316 CZ3	TRP	684	11.322 9.022 25.315 1 00 41 2-
ON 5	5317 CH2	TRP	684	43 8.576 27.692 1 00 4
			- •	43.917 8 933 1.00 41.99
SSSD/55145	-			26.541 1.00 41.07
~~~~, 33 14 5	o ν/11			



ATOM	5318	С	TRP	684	49.964	6.125	25.115	1.00 36.12
ATOM	5319	0	TRP	684	49.152	5.410	24.511	1.00 38.69
ATOM	5320	N	SER	685	51.029	6.690	24.534	1.00 33.48
ATOM	5322	CA	SER	685	51.395	6.491	23.130	1.00 26.49
ATOM	5323	CB	SER	685	52.636	7.300	22.802	1.00 23.40
MOTA	5324	OG	SER	685	52.403	8.688	22.992	1.00 30.31
ATOM	5326	С	SER	685	51.665	5.015	22.859	1.00 26.25
MOTA	5327	0	SER	685	51.377	4.510	21.782	1.00 28.78
ATOM	5328	N	PHE	686	52.214	4.319	23.846	1.00 28.14
MOTA	5330	CA	PHE	686	52.470	2.884	23.727	1.00 28.53
ATOM	5331	CB	PHE	686	53.245	2.399	24.947	1.00 27.34
MOTA	5332	CG	PHE	686	53.567	0.937	24.917	1.00 29.91
MOTA	5333	CD1		686	54.424	0.419	23.942	1.00 29.23
ATOM	5334		PHE	686	53.016	0.075	25.861	1.00 28.28
MOTA	5335		PHE	686	54.725	-0.936	23.908	1.00 27.65
ATOM	5336	CE2		686	53.307		25.840	1.00 27.18
ATOM	5337	CZ	PHE	686	54.166	-1.787	24.861	1.00 30.06
MOTA	5338	C	PHE	686	51.129	2.117	23.618	1.00 31.42
MOTA	5339	0	PHE	686	51.041	1.096	22.930	1.00 29.05
ATOM	5340	И	GLY	687	50.093	2.623	24.298	1.00 31.18
ATOM	5342	CA	GLY	687	48.783	2.000	24258	1.00 32.16
ATOM	5343	C	GLY	687	48.276	2.026	22.825	1.00 35.09
ATOM	5344	0	GLY	687	47.805	1.011	22.289	1.00 36.38
MOTA	5345	Ŋ	VAL	688	48.378	3.188	22.186	1.00 33.72
ATOM	5347	CA	VAL	688	47.949	3.307	20.808	1.00 30.28
MOTA	5348	CB	VAL	688	47.996	4.761	20.322	1.00 28.62
ATOM	5349		VAL	688	47.433	4.862	18.905	1.00 26.79
ATOM	5350	CG2	VAL	688	47.202	5.645	21.275	1.00 26.40
MOTA	5351	Ç	VAL	588	48.823	2.406	19.930	1.00 30.01
ATOM	5352	0	VAL	688	48.324	1.782	18.989	1.00 30.37
ATOM	5353	N	LEU	689	50.108	2.282	20.273	1.00 29.76
ATOM	5355	CA	LEU	689	51.022	1.418	19.510	1.00 29.37
ATOM ATOM	5356	CB CG	LEU	689	52.476	1.577	19.982	1.00 25.78
ATOM	5357 5358		LEU	689	53.564	0.944	19.097	1.00 23.00
ATOM	5359		LEU	689	54.855	1.741	19.153	1.00 24.44 1.00 21.63
ATOM	5360	CD2	LEU	689 689	53.823	-0.471	19.479	
ATOM	5360	0	LEU	689 689	50.583 50.708	-0.043 -0.806	19.634 18.678	1.00 29.98 1.00 28.75
ATOM	5362	N	LEU	690	50.708	-0.409	20.803	1.00 28.75
ATOM	5364	CA	LEU	690	49.562	-1.764	21.060	1.00 32.36
ATOM	5365	CB	LEU	690	49.362	-1.929	22.517	1.00 32.88
ATOM	5366	CG	LEU	690	50.107	-2.192	23.658	1.00 32.33
ATOM	5367		LEU	690	49.330	-2.201	24.962	1.00 32.00
ATOM	5368		LEU	690	50.834	-3.513	23.475	1.00 30.74
ATOM	5369	C	LEU	690	48.369	-2.018	20.156	1.00 30.78
ATOM	5370	0	LEU	690	48.248	-3.079	19.550	1.00 35.08
ATOM	5370	N	TRP	691	47.490	-1.026	20.065	1.00 34.28
ATOM	5373	CA	TRP	691	46.304	-1.026	19.221	1.00 34.28
ATOM	5374	CB	TRP	691	45.483	0.172	19.221	1.00 33.79
ATOM	5375	CG	TRP	691	44.147	0.172	18.669	1.00 32.68
ATOM	5376	CD2		691	43.888	0.490	17.312	1.00 31.23
ATOM	5377	CE2		691	42.506	0.310		
	J J I I	CDZ	INP	UDI	14.500	0.310	17.089	1.00 29.96

A'.	rom	5378	CE3	TRP 691	
	TOM	5379	CD1		44.686 0.949 16.257 1.00 28.70
	OM !	5380	NE1		10.225 19.208 1.00 29 27
	OM !	5382	CZ2		41.951 -0.130 18 265 1 00 25
ΓA	'OM	5383	-		41.909 0.555 15.845 1.00 00
AT		384	_		44.093 1.194 15.021 1.00 29.50
AT		385			42.719 1.002 14 830 1.00 27.43
AT		386	_		46.744 -1.319 17 763 1 00 29.27
ATO		387			46.139 -2.088 17.029 2.00 34.12
ATO		389		LU 692	47.817 -0.626 1.00 33.88
ATO		390		LU 692	48.355 -0.722 -1.00 36.37
ATO		391		LU 692	49.532 0.332
ATO				ւՄ 692	49 138 3 501
ATO		392	CD GI		50.318 2.505
ATO		393	OE1 GI		51.150 2.047 1.00 35.28
ATO		394	OE2 GI		50.430 3 222 1.00 37.81
ATO			C GL	U 692	48.810 3.112 14.237 1.00 34.85
ATO			O GL	U 692	48 500 2.118 15.658 1.00 35.71
ATO			N IT	E 693	49 430 14.544 1.00 37.26
			CA IL	E 693	19 044 16.610 1.00 35.05
ATO			CB IL		50.043 16.396 1.00 35.00
ATON			G2 IL		51 275
MOTA	_		G1 IL	E 693	53 003 17.400 1.00 36.03
ATOM			D1 ILE	693	52 014 17.669 1.00 34.66
ATOM		_	LLE		48 810
ATOM		)5 C	ILE		18 700 16.232 1.00 34.29
ATOM		)6 N	PHE		3,943 15,281 1,00 33 66
ATOM		_	A PHE		3.079 17.127 1.00 34 44
ATOM	540	9 C	в рне		16 156
ATOM	541	0 C		694	18.490 1 00 35 36
ATOM	541		D1 PHE	694	47.158 -6.787 19.428 1.00 35 36
ATOM	541	2 CI	D2 PHE	694	47.796 -6.017 20.389 1 00 33 07
ATOM	541		E1 PHE	694	47.574 -8.111 19.237 1.00 31 74
ATOM	5414	4 CE		694	48.837 -5.539 21.137 1.00 31 01
ATOM	5415	5 Cz		694	48.614 -8.643 19.982 1.00 31 64
ATOM	5416	5 C	PHE	694	49.254 -7.855 20 934 1 00 3-
ATOM	5417		PHE	694	45.688 -5.771 15 986 1 00 75
MOTA	5418		THR	695	44.844 -6.632 15 729 1 00 75 -
ATOM	5420				45.781 -4.626 15.313 1 00 35 76
ATOM	5421		THR	695	44.898 -4.331 14.191 1.00 34.86
ATOM	5422		1 THR	695	44 745 2 22
MOTA	5424		2 THR	695	45.246 -1.909 14 211
ATOM	5425	C.	THR	695	43.497 -2.795 15 603 1 00 31.61
ATOM	5426	o		695	45.766 -4.426 12 934 1 00 25
ATOM	5427	N	THR	695	45.333 -4.064 11 841 1 00 33.95
ATOM	5429		LEU	696	46 993
ATOM	5430	CA	LEU	696	47 979 5 300
ATOM	5431	CB	LEU	696	47 622 6 204
ATOM		CG	LEU	696	47 493 7 657
ATOM	5432	CD1	LEU	696	47 315 0 73
ATOM	5433		LEU	696	48 719 7 025
ATOM	5434	C	LEU	696	48 280 3 276
	5435	0	LEU	696	48 259 2 225
ATOM	5436	N	GLY	697	48 597 3 757
					48.597 -2.768 11.867 1.00 33.65

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-1.529 ATOM 5438 CA GLY 697 48.940 11.188 1.00 32.78 MOTA 5439 GLY 697 47.742 -0.641 10.960 1.00 33.06 С 697 47.728 10.048 MOTA 5440 0 GLY 0.172 1.00 34.74 5441 698 46.719 -0.798 11.782 ATOM N GLY 1.00 35.53 GLY 11.612 ATOM 5443 CA 698 45.531 0.009 1.00 36.87 ATOM 5444 C GLY 698 45.771 1.496 11.753 1.00 34.92 **ATOM** 5445 0 GLY 698 46.779 1.926 12.299 1.00 34.08 ATOM 5446 SER 699 44.814 2.271 11.265 1.00 36.45 Ν **ATOM** 5448 CA SER 699 44.858 3.725 11.318 1.00 35.36 MOTA 5449 CB SER 699 44.363 4.290 9.995 1.00 34.58 MOTA 5450 OG SER 699 44.126 5.684 10.087 1.00 41.43 **ATOM** 5452 С SER 699 43.927 4.146 12.451 1.00 36.53 MOTA 5453 0 SER 699 42.734 3.812 12.438 1.00 37.58 ATOM 5454 PRO 700 N 44.471 4.799 13.491 1.00 36.03 ATOM 5455 CD PRO 700 45.896 5.028 13.776 1.00 34.58 ATOM 5456 CA PRO 700 43.630 5.228 14.611 1.00 35.47 ATOM 5457 CB PRO 700 44.655 5.573 15.694 1.00 34.59 **ATOM** 5458 CG PRO 700 45.840 5.990 14.919 1.00 34.18 ATOM 5459 С PRO 700 42.742 6.411 14.247 1.00 34.66 ATOM 5460 0 PRO 700 43.194 7.363 13.616 1.00 34.39 ATOM 5461 N TYR 701 41.462 6 293 14.588 1.00 34.11 40.459 **ATOM** 5463 CA TYR 701 7.324 14.338 1.00 33.11 ATOM 5464 CB TYR 701 40.713 8..548 15.225 1.00 38.13 ATOM 5465 CG TYR 701 40.552 16.706 8.272 1.00 43.52 ATOM 5466 CD1 TYR 701 8.637 17.616 41.538 1.00 14.79 **ATOM** 1.00 49.99 546? CE1 TYR 701 41.387 8.391 18.978 MOTA 54*E*8 CD2 TYR 701 1.00 47.59 . 39.405 7.647 17.197 MOTA 5469 CE2 TYR 701 39.245 7.395 18.552 1.00 49 15 MOTA 5470 CZTYR 701 40.237 7.770 19.444 1.00 50.84 ATOM TYR 5471 701 OH 40.091 7.539 20.804 1.00 54.00 MOTA 701 5473 C. TYR 40.389 7.736 12.877 1.00 30.95 40.597 8.900 **ATOM** 5474 TYR 701 12.534 O 1.00 30.64 **ATOM** 5475 702 6.773 N PRO 40.096 11.985 1.00 30.06 ATOM 5476 39.887 CD PRO 702 5.336 12.192 1.00 25.47 ATOM 5477 CA PRO 702 40.014 7.112 10.561 1.00 29.36 ATOM 5478 702 CB PRO 39.836 5.744 9.899 1.00 25.86 MOTA 5479 CG PRO 702 39.185 4.946 10.929 1.00 24.42 MOTA 5480 C PRO 702 38.859 8.045 10.256 1.00 31.49 MOTA 5481 0 PRO 702 37.716 7.794 10.654 1.00 33.50 MOTA 5482 GLY 703 39.194 N 9.151 9.592 1.00 30.85 MOTA 5484 CA GLY 703 38.210 10.149 9.212 1.00 27.67 ATOM 703 5485 С GLY 37.9B5 11.230 10.250 1.00 27.39 ATOM 5486 GLY 703 0 37.270 12.194 9.981 1.00 26.56 ATOM 5487 N VAL 704 38.627 11.100 11.412 1.00 27.05 **ATOM** 5489 CA VAL 704 38.466 12.053 12.505 1.00 28.50 ATOM 5490 CB VAL 704 38.576 11.364 13.876 1.00 28.95 ATOM 5491 CG1 VAL 704 38.509 12.397 14.990 1.00 29.36 MOTA 5492 CG2 VAL 704 37.475 10.338 14.045 1.00 29.64 **ATOM** 5493 C VAL 704 39.473 13.194 12.493 1.00 30.95 MOTA 5494 0 VAL 704 40.669 12.977 12.661 1.00 32.90 MOTA 5495 N PRO 705 39.001 14.428 12.269 1.00 31.09 MOTA 5496 CD PRO 705 37.682 14.795 11.728 1.00 31.49



חת	POM.					
	rom	5497		PRO	705	5 39.926 15.561 12.255
		5498		PRO	705	13.561 12.255 1 00 29 66
	OM	5499	CG	PRO	705	10.018 11.477 1 00 20 16
		5500	C	PRO	705	37.720 16.289 11 770 1 22
AT		5501	0	PRO		40.334 16.028 13.654
AT		5502		VAL	705	39.693 15.695 14.659 1.00
ATO		5504			706	41.396 16.828 13.690 1.00 24.77
ATO		505		VAL	706	41,976 12 255
ATO		506		VAL	706	43.023 19.450
ATC		507	CG1	VAL	706	43.680 18.003
ATC			CG2 1		706	44.058 17.042
ATO		508	C /	/AL	706	10 077 17, 942 13.653 1.00 37 26
ATO		509	0 I	'AL	706	41 050 15.943 1.00 38 21
		510	И G	Lυ	707	10 000 17.130 1.00 37 65
ATO		512	CA G	LU	707	15.467 1 00 40 00
ATO		513	CB G	LU	707	15.380 16.324 7 00 40 55
ATO		314	C G	LU	707	38.186 20.324 15.499 1 00 10 56
ATO	M 55	15	_	ւՄ	707	38.164 18.288 16 950 1 00
MOTA		16		LU LU		37.871 18.323 18 150
ATOM	1 55	18		T.D.	708	37.784 17.311 16 143 1 20
ATOM		19			708	36 947 16 220
ATOM	1 55				708	36 509 15 700
ATOM	_				708	35 687 16 372
АТОМ					708	34.511 16 001
ATOM			OE1 GL	U	708	33.856 16.242 4.00 55.51
ATOM			DE2 GL		708	34.244 19.000 13.699 1.00 58.91
ATOM			GL		708	37.661 35 333
ATOM			) GL	U .	708	37 050 71 17.598 1.00 44.63
ATOM	552	_	I LE	י ד	709	38 360 15 18.585 1.00 45.12
	552		A LE	J	09	39 700 13.141 17.390 1.00 43.72
ATOM	552	-	B LE	7	09	14.345 18.312 1.00 10 05
ATOM	553		G LE		09	14.243 17.823 1 00 24 00
ATOM	553	1 C	D1 LEU	_	09	13.359 18.756 1 00 3" 00
ATOM	553:		D2 LEU		09	41.019 11.918 18.598 1.00 39 30
ATOM	553	3 C	LEU		09	43.495 13.533 18.454 1 00 21 10
ATOM	5534	4 0	LEU	•		39.751 15.001 19.683 1.00 25
ATOM	5535		PHE	•	09	39.646 14.317 20 714 1 00 37.26
ATOM	5537				LO	39.872 16.327 19.697 1.00 37.71
ATOM	5538			7:		39.862 77.060
ATOM	5539			71		40.016 10.555
ATOM	5540			71		41 383 10 050
ATOM	5541		1 PHE	71		42 441 10 045
ATOM	5542	CD	2 PHE	71		41 621 20 20 20 2 1.00 47.07
ATOM	5543	CE	1 PHE	71		43 716 10 42.91
ATOM			2 PHE	71	0	42.890 20 500 1.00 49.22
ATOM	5544	CZ	PHE	71	0	43 942 10 600
	5545	C	PHE	71		39.569 19.881 19.307 1.00 48.40
ATOM	5546	0	PHE	71		39 503 10.787 21.698 1.00 43 80
ATOM	5547	N	LYS	71:		22.904 1.00 44 54
ATOM	5549	CA	LYS	711		37.452 16.790 20.968 1.00 44 15
ATOM	5550	CB	LYS			36.148 16.539 21.569 1 00 42 60
ATOM	5551	CG	LYS	711		35.029 16.855 20 577 1 00
MOTA	5552	CD	LYS	711		33.661 16.781 21 200 1 20
	5553	CE		711		32.560 17.205 20 262 1.00
3	5554	NZ	LYS	711		31.212 16.804 20 855 1 22 7
		147	LYS	711		30 078 17 000 20.833 1.00 50.61
						30.078 17.204 19.987 1.00 56.56

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ATOM 5558 C LYS 711 36.045 15.105 22.084 1.00 41.50 MOTA 5559 0 LYS 35.589 711 14.875 23.202 1.00 41.06 MOTA 5560 N LEU 712 36.489 14.144 21.282 1.00 41.61 **ATOM** 5562 CA LEU 712 36.463 12.737 21.687 1.00 43.22 MOTA 5563 CB LEU 712 37.070 11.841 20.600 1.00 41.69 **ATOM** 5564 CG LEU 712 36.246 11.404 19.397 1.00 38.07 ATOM 5565 CD1 LEU 37.071 712 10.460 18.527 1.00 34.55 MOTA 5566 CD2 LEU 712 34.990 10.714 19.891 1.00 37.28 **ATOM** 5567 С LEU 37.253 12.536 712 22.982 1.00 43.94 **ATOM** 5568 LEU 712 0 36.804 11.832 23.900 1.00 41.71 ATOM 5569 N LEU 713 38.444 13.129 23.029 1.00 45.26 MOTA 5571 CA LEU 713 39.318 13.022 24.191 1.00 46.47 MOTA 5572 CB LEU 713 40.647 13 728 23.925 1.00 46.32 MOTA 5573 CG LEU 713 41.524 13.012 22.889 1.00 44.05 MOTA 5574 CD1 LEU 713 42.853 13.737 22.734 1.00 39.96 5575 MOTA CD2 LEU 713 41 758 11.571 23.328 1.00 41.78 ATOM 5576 С LEU 713 38.665 13.519 25.477 1.00 47.50 ATOM 5577 С LEU 713 38.630 12.789 26.472 1.00 48,26 **ATOM** 5578 N LYS 714 38.098 14.725 25.440 1.00 47.08 **ATOM** 5580 CA LYS 714 37.419 . 15.302 26.600 1.00 45.59 **ATOM** 5581 СВ LYS 714 36.974 16.727 26.293 1.00 47.53 ATOM 5582 CG LYS 714 38.126 17.661 26.064 1.00 51.33 ATOM 5583 CDLYS 714 37.647 19.044 25.689 1.00 59.12 **ATOM** 5584 CE LYS 714 38.836 19.917 25.273 1.00 64.39 ATOM 5585 NZ. LYS 714 39.843 20.072 26.370 1.00 66.31 MOTA 5589 C 714 36.217 14.476 LYS 27.056 1.00 44.19 MOTA 5590 0 LYS 714 35.895 14.447 28.244 1.00 43.04 MOTA 5591 Ŋ GLU 715 35.565 13.805 26.112 1.00 43.89 12:976 MOTA 5593 CA GLU 715 34.401 26.424 1.00 44.12 MOTA 5594 CB GLU 715 33.512 12.785 25.190 1.00 47.40 MOTA 5595 715 . CG GLU 32.860 14.053 24.623 1.00 52.31 ATOM 5596 CD GLU 715 31.953 13.763 23.427 1.00 56.22 **ATOM** OE1 GLU 5597 715 32.121 12.699 22.784 1.00 57.16 **ATOM** 5598 OE2 GLU 715 31.059 14.588 23.138 1.00 57.32 **ATOM** 5599 C. GLU 715 34.809 11.605 26.956 1.00 42.47 MOTA 5600 GLU 715 33.964 0 10.718 27.094 1.00 41.03 MOTA 5601 N GLY 716 36.101 11.419 27.201 1.00 41.06 MOTA 5603 CA GLY 716 36.593 27.718 10.150 1.00 41.58 MOTA 5604 С GLY 716 36.548 8.985 26.739 1.00 41.60 MOTA 5605 0 GLY 716 36.640 7.816 27.141 1.00 38.34 MOTA 5606 N HIS 717 36.469 9.303 25.450 1.00 42.80 MOTA 5608 CA HIS 717 36.398 8.278 24.420 1.00 45.03 **ATOM** 5609 CB HIS 717 36.082 8.894 23.052 1.00 46.28 ATOM 5610 CG HIS 717 35.987 7.887 21.940 1.00 48.73 MOTA 5611 CD2 HIS 717 34.941 7.157 21.483 1.00 48.67 MOTA 5612 ND1 HIS 717 37.071 7.521 21.169 1.00 49.33 ATOM 5614 CE1 HIS 717 36.701 6.607 20.290 1.00 45.65 **ATOM** 5615 NE2 HIS 717 35.410 6.370 20.460 1.00 45.87 ATOM 5617 С HIS 717 37.662 7.448 24.324 1.00 46.84 MOTA 5618 0 HIS 717 38.767 7.980 24.319 1.00 48.06 ATOM 5619 N ARG 718 37.478 6.138 24.217 1.00 48.75 **ATOM** 5621 CA ARG 718 38.573 5.181 24.091 1.00 49.16

	ATOM	562	2 CB	ARG	718	
	MOTA	562	G CG	ARG	718	4.345 25 370
	TOM	5624	CD	ARG	718	39.005 5.164 26 612
	TOM	5625	NE	ARG	718	5.891 26 474
	TOM	5627	CZ	ARG	718	40.724 6.639 27 672
	TOM	5628	NHl		718	40.598 7.961 27 912
	TOM	5631	NH2	ARG		40.094 8.705 26 926
	rom	5634	_	ARG	718	41.025 8.553 28 820
	MOT	5635	_	ARG	718	38.257 4.293 22 870
ΓA		5636			718	37.086 4.003 05 1.00 50.73
AT		5638	`	MET	719	39.286 3.000 22.001 1.00 51.78
AT		639		/ET	719	39.086
AT	~	640		ET	719	40.355 3.013 20 1.00 50.56
AT	_	641	~-	ET	719	40.748 4 335 20.094 1.00 48.85
ATO	~	642		ET	719	42 152 19.438 1.00 45 25
ATO	~~	643	_	ET	719	43 471 18.335 1.00 43 24
ATC			_	ET	719	39 640 19.465 1.00 36 42
ATO	_	644		ET	719	39 007 21.312 1.00 51 07
ATO	-	645		SP	720	37 707
. ATO	•	547	CA A		720	37 254 20.462 1.00 53 92
ATO		548	CB AS	SP	720	20.548 1 00 55 00
ATO		49	CG AS	P	720	24 000 17.553 1.00 57 16
		50	OD1 AS	P ·	720	0.320 19.552 1 00 50 55
ATON		51	OD2 AS		720	1.316 20.312 1 00 62 0
ATON			C AS		20	0.042 18.758 1 00 54 75
ATOM	_		O AS		20	38.326 -1.343 20.638 1 00 55 00
ATOM		54	V LY		21	33.397 -1.190 20.027 1 00 55 00
ATOM		56 (	A LY	_ `	21	38.008 2.450 21.304 1.00 56.20
ATOM			B Lys		21	30.892 -3.605 21 370
MOTA		58 C	G LYS		21	30.344 -4.606 22 270 -
ATOM		i9 c	D LYS		21	39.005 -5.977 22 336
ATOM	566	0 0	E LYS			30.4496.873 23 403 - 32.49
ATOM	566	1 N				38.474 -8.329 22 905
ATOM	566	5 C	LYS			38.107 -9.194 24 156
ATOM	566	6 O	LYS			38.930 -4.241 19 905
ATOM	566		PRO	72		37.884 -4.532 19.403
ATOM	566			72		40.133 -4.439 19 423
ATOM	5669			72		41.461 -3.968 19.036
ATOM	5670			72.		40.208 -5.046 18.004
ATOM	5671			72:		41.702 -4 953 1.00 51.82
ATOM	5672	_	PRO	722		42.143 -3.768 18.503
ATOM	5673	_		722		39.765 -6 400 10.301 1.00 49.06
ATOM	5674		PRO	722		39.678 -7 130 18.123 1.00 50.10
ATOM	5676		SER	723		39.453 -7.020 13.188 1.00 48.82
ATOM	5677	_	SER	723		39.079 -R 410 - 10.945 1.00 49.87
ATOM	5678	CB	SER	723		38.396 -9.642 1.00 50.27
ATOM		OG	SER	723		39.273 -9.333 1.00 48.56
ATOM	5680	C	SER	723		40.414 -9.744 1.00 48.93
ATOM	5681	0	SER	723		41,400 0 572 1.00 51.33
ATOM	5682	N	ASN	724		40 445 10.079 16.311 1.00 51 10
ATOM	5684	CA	ASN	724		41 673 17.551 1.00 54 65
ATOM	5685	СВ	ASN	724		42 270 -1.002 17.706 1.00 56 76
ATOM	5686	CG	ASN	724		41 600 15.359 1.00 58 96
MOTA	5687	OD1	ASN	724		
						41.645 -13.508 15.948 1.00 67.56

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MOTA	5688	ND2	ASN	724	41.154	-11.960	14.403	1.00 60.12
MOTA	5691	С	ASN	724	42.622	-10.381	18.683	1.00 57.26
ATOM	5692	0	ASN	724	43.786	-10.131	18.383	1.00 58.40
MOTA	5693	N	CYS	725	42.089	-10.045	19.845	1.00 57.58
MOTA	5695	CA	CYS	725	42.852	-9.418	20.908	1.00 57.02
MOTA	5696	CB	CYS	725	42.835	-7.885	20.803	1.00 55.65
MOTA	5697	SG	CYS	725	43.782	-7.034	22.119	1.00 52.17
MOTA	5698	C	CYS	725	42.158	-9.884	22.177	1.00 56.53
MOTA	5699	0	CYS	725	40.927	-9.954	22.240	1.00 55.99
MOTA	5700	N	THR	726	42.957	-10.279	23.155	1.00 56.09
ATOM	5702	CA	THR	726	42.453	-10.773	24.423	1.00 57.09
ATOM	5703	CB	THR	726	43.551	-11.579	25.129	1.00 57.12
MOTA	5704	OG1	THR	726	44 588	-10.696	25.562	1.00 59.14
ATOM	5706	CG2	THR	726	44.152	-12.587	24.154	1.00 55.09
ATOM	5707	C	THR	726	41.994	-9.608	25.288	1.00 57.58
MOTA	5708	0	THR	726	42.555	-8.518	25.195	1.00 58.49
MOTA	5709	N	ASN	727	40.979	-9.832	26.120	1.00 58.48
MOTA	5711	CA	ASN	<b>7</b> 27	40.482	-8.774	26.986	1.00 58.74
MOTA	5712	CB	ASN	727	39.331	-9.267	27.864	1.00 66.81
ATOM	5713	CG	ASN	727	39.674	-10.534	28.631	1.00 76.72
ATOM	5714	OD1	ASN	727	40.778	-10.689	29.161	1.00 80.48
ATOM	5715	ND2	ASN	727	38.716	-11.458	28.689	1.00 82.39
ATOM	5718	C	ASN	727	41.606	-8.238	27.852	1.00 55.48
ATOM	5719	0	ASN	727	41.589	-7.080	28.255	1.00 51.24
MOTA	5720	N	GLU	728	42.589	-9.099	28.114	1.00 55.37
ATOM	5722	CA	GLU	728	43.757	-8.739	28.913	1.00 55.53
MOTA	5723	CB	GLU	728	44.611	-9.983	29.198	1.00 55.75
ATOM	5724	CG	GLU	728	45.881	-9.699	30.006	1.00 58.24
ATOM	5725	CD	GLU	728	46.606	-10.958	30.463	1.00 58.16
ATOM	5726	OE1	GLU	728	46.977	-11.796	29.611	1.00 56.39
ATOM	5727	OE2	GLU	728	46.816	-11.102	31.686	1.00 58.35
MOTA	5728	C	GLU	728	44.564	-7.685	28.153	1.00 54.11
MOTA	5729	0	GLU	728	44.790	-6.575	28.654	1.00 55.67
ATOM	5730	N	LEU	729	44.954	-8.020	26.926	1.00 49.65
MOTA	5732	CA	LEU	729	45.715	-7.106	26.086	1.00 46.10
MOTA	5733	CB	LEU	729	46.038	-7.766	24.742	1.00 39.77
ATOM	5734	CG	LEU	729	47.136	-8.836	24.848	1.00 36.12
ATOM	5735	CD1	LEU	729	47.118	-9.757	23.673	1.00 34.89
ATOM	5736	CD2	LEU	729	48.498	-8.193	24.987	1.00 33.47
ATOM	5737	C	LEU	729	44.950	-5.794	25.908	1.00 45.05
ATOM	5738	0	LEU	729	45.522	-4.713	26.019	1.00 45.58
ATOM	5739	N	TYR	730	43.640	-5.884	25.722	1.00 43.53
MOTA	5741	CA	TYR	730	42.831	-4.692	25.557	1.00 43.57
ATOM	5742	CB	TYR	730	41.414	-5.064	25.097	1.00 41.49
ATOM	5743	CG	TYR	730	40.492	-3.870	24.951	1.00 40.28
ATOM	5744	CD1	TYR	730	40.763	-2.865	24.013	1.00 36.86
MOTA	5745	CE1	TYR	730	39.937	-1.752	23.891	1.00 36.21
ATOM	5746	CD2	TYR	730	39.361	-3.730	25.768	1.00 39.44
ATOM	5747	CE2	TYR	730	38.522	-2.616	25.654	1.00 38.13
MOTA	5748	CZ	TYR	730	38.817	-1.632	24.712	1.00 38.79
ATOM	5749	OH	TYR	730	37.974	-0.542	24.575	1.00 40.32
ATOM	5751	С	TYR	730	42.806	-3.866	26.856	1.00 44.45

Δ.	MOT	E 7 C /				
	TOM	5752		TYR	730	42.786 -2.632 26 812
	TOM	5753		MET	731	42 700 -2.632 26.818 1.00 43 45
		5755	_	MET	731	2.534 28.006 1 00 46 44
	TOM	5756		MET	731	42.805 -3.812 29.279 1 00 48 52
	TOM	5757	CG	MET	731	42.516 -4.748 30.447 1.00 54.60
A:	TOM	5758	SD	MET		41.132 -5.387 30 300 1 00
	<b>TOM</b>	5759	CE	MET	731	39.781 -4.189 30 303
rA		5760			731	39.492 -4 010 1.00 /0.49
		5761	_	MET	731	44.167 -3 132 1.00 72.27
		5762		MET	731	44.280 -2 005 1.00 46.48
		5764		MET	732	45.202 -2 752
AT				MET	732	46 530 3.731 28.881 1.00 43 80
AT		765		MET	732	47 503 3.167 28.939 1.00 43.03
	_	766	CG 1	ÆT	732	4.104 28.322 1 00 20 4.
AT(		767	SD N	1ET	732	28.427 1 00 36 02
ATO		768	CE N	ET	732	50.312 -4.775 27.979 1 00 36 47
ATC	_	769		ET	732	30.54/ ~5 573 29 530
ATC	)M 5	770		ET		46 474 1.833 28 188
ATO		771			732	46.995 -0.827 28.650 - 1.00 42.08
ATO		773			733	45.775
ATO		774			733	45.608 -0.500 -1.00 43.14
ATO		775			733	44.852 -0.977 1.00 42.24
ATO!	,		CG MI		733	45.607 1 710 24.947 1.00 41.41
ATO			SD MI		733	44 560 23.938 1.00 40.23
ATON			CE ME	e <b>t</b>	733	45 100 22.419 1.00 38 05
	_		C ME	T ;	33	14 220 3.724 21.982 1.00 28 12
ATOM			O ME	T 7	33	27.074 1.00 41.60
ATOM	,	80 I	v ar	_	34	1.550 27.196 1.00 42.70
ATOM		82 (	A AR		34	43./13 -0.053 27 605
ATOM		33 c	B AR	-	34	44.893 0.839 28 462 3
ATOM		34 C	G AR	_ `	34	*1.042 0.119 29 366
ATOM		15 C	D ARC	_		40.753 -0.374 27 852 11 -
ATOM	578				34	40.360 0.763 26 960 39.76
ATOM	578				34	39.535 1.745 27.652
ATOM	578		H1 ARG		34	38.207 1 603
ATOM	579		III ARG			37.542 0.700 1.00 50.22
ATOM	579		H2 ARG		4	37.534 2.642 27.11/ 1.00 51.18
ATOM	579e		ARG			43,719 1 305 20.346 1.00 53.24
ATOM			ARG		4	43 610 1.365 29.630 1.00 42 42
ATOM	5797		ASP	73	5	44 501 29.969 1.00 42 59
АТОМ	5799			73	5	45 464 30.187 1.00 41 40
	5800		ASP	73		46 327 31.286 1.00 43 33
ATOM	5801			73		0.134 31 755 1 00 15
ATOM	5802		1 ASP	735	-	1.256 32.496 1 00 54 05
ATOM	5803	OD	2 ASP	735		2.451 32.322 1 00 53 40
ATOM	5804	С	ASP			44.612 -0.900 33 245
ATOM	5805	0	ASP	735		46.365 2.107 30 840 3 35.59
ATOM	5806	N	CYS	735		46.484 3.124 31 542 1 72
ATOM	5808	CA		736		47.021
ATOM	5809		CYS	736		47.896 3.052
ATOM	5810	CB	CYS	736		48.545 2.460 = 1.00 35.90
ATOM		SG	CYS	736		49.634 1.007 27.858 1.00 33.62
ATOM	5811	C	CYS	736		47 100 28.104 1.00 33 92
ATOM	5812	0	CYS	736		47 653 4.208 28.855 1.00 35.96
	5813	N	TRP	737		45 702 28.830 1.00 35.59
ATOM	5815	CA	TRP	737		45.793 4.039 28.668 1.00 38.00
						44.906 5.156 28.372 1.00 40.14
SSSDVECT						

ATOM	5816	CB	TRP	737	43.910	4.766	27.274	1.00 40.93
MOTA	5817	CG	TRP	<b>7</b> 37	44.563	4.379	25.977	1.00 42.36
ATOM	5818	CD2	TRP	737	44.018	3.518	24.969	1.00 43.84
ATOM	5819	CE2	TRP	737	44.972	3.437	23.929	1.00 46.42
MOTA	5820	CE3	TRP	737	42.817	2.806	24.845	1.00 42.43
ATOM	5821	CD1	TRP	737	45.793	4.775	25.519	1.00 42.57
ATOM	5822	NE1	TRP	737	46.043	4.214	24.292	1.00 44.22
ATOM	5824	CZ2	TRP	737	44.756	2.666	22.773	1.00 44.97
MOTA	5825	CZ3	TRP	737	42.606	2.042	23.699	1.00 40.74
ATOM	5826	CH2	TRP	737	43.571	1.978	22.682	1.00 40.75
MOTA	5827	C	TRP	737	44.157	5.706	29.584	1.00 40.62
ATOM	5828	О	TRP	737	43.085	6.285	29.437	1.00 41.37
ATOM	5829	N	HIS	738	44.706	5.533	30.783	1.00 42.09
MOTA	5831	C'A	HIS	738	44.044	6.059	31.966	1.00 43.78
ATOM	5832	CB	HIS	738	44.635	5.463	33.248	1.00 46.52
MOTA	5833	CG	HIS	738	43.878	5.844	34.486	1.00 52.24
MOTA	5834	C.D.5	HIS	738	43.599	7.053	35.025	1.00 50.95
$\Lambda$ TOM	5835	ND1	HIS	738	43.271	4.914	35.299	1.00 56.16
ATOM	5837	CEI	HIS	738	42.643	5.536	36.285	1.00 57.23
MOTA	5838	NE3	HIS	738	42.827	6.835	36.141	1.00 53.22
ATOM	5840	C	HIS	738	44.183	7.577	31.964	1.00 42.81
ATOM	5841	0	HIS	738	45.235	8.093	31.654	1.00 42.12
MOTA	5842	N	ALA	739.	43.121	8.285	32.324	1.00 45.66
ATOM	5844	CA	ALA	739	43.130	9.750	32.350	1.00 49.42
MOTA	5845	CB	ALA	739	41.739	10.262	32.681	1.00 53.04
ATOM	5846	C	ALA	739	44.167	10.380	33.291	1.00 50.18
ATOM	5847	O	ALA	739 .	44.710	11.450	33.006	1.00 51.86
MOTA	5848	N	VAL	740	44.322	9.780	34.466	1.00 49.96
ATOM	5850	CA	VAL	740	45.299	10.219	35.467	1.00 50.17
ATOM	5851	CB	VAL	740	44.828	9.849	36.881	1.00 50.33
MOTA	5852	CG1	VAL	740	45.880	10.209	37.896	1.00 51.40
ATOM	5853		VAL	740	43.534	10.559	37.193	1.00 50.86
ATOM	5854	С	VAL	740	46.626	9.497	35.196	1.00 49.81
ATOM	5855	0	VAL	740	46.749	8.295	35.472	1.00 49.85
ATOM	5856	N	PRO	741	47.646	10.230	34.713	1.00 47.92
ATOM	5857	CD	PRO	741	47.618	11.683	34.476	1.00 46.97
MOTA	5858	CA	PRO	741	48.968	9.686	34.393	1.00 46.47
ATOM	5859	CB	PRO	741	49.796	10.941	34.134	1.00 44.38
ATOM	5860	CG	PRO	741	48.800	11.877	33.561	1.00 44.86
ATOM	5861	С	PRO	741	49.593	8.815	35.480	1.00 47.21
ATOM	5862	0	PRO	741	50.243	7.816	35.176	1.00 46.77
ATOM	5863	N	SER	742	49.380	9.181	36.741	1.00 48.87
ATOM	5865	CA	SER	742	49.939	8.430	37.860	1.00 50.19
ATOM	5866	CB	SER	742	49.753	9.203	39.166	1.00 51.87
ATOM	5867	OG	SER	742	48.389	9.514	39.391	1.00 54.19
ATOM	5869	C	SER	742	49.331	7.040	38.010	1.00 51.30
ATOM	5870	0	SER	742	49.863	6.192	38.723	1.00 51.14
ATOM	5871	N	GLN	743	48.207	6.814	37.343	1.00 53.07
ATOM	5873	CA	GLN	743	47.531	5.531	37.414	1.00 53.50
ATOM	5874	CB	GLN	743	46.015	5.745	37.548	1.00 59.34
ATOM	5875	CG	GLN	743	45.412	5.307	38.898	1.00 66.19
ATOM	5876	CD	GLN	743	46.133	5.896	40.106	1.00 70.07

	TOM	5877	OE1	GLN	743	<b>.</b>
	TOM	5878	NE2	GLN	743	5.170 40 005 -
	TOM	5881	C	GLN	743	7 46.047 7.209 40 273 3 55
	TOM	5882	0	GLN	743	47.850 4.613 36 226 1 22
		5883	N	ARG	744	47.504 3.425 36 360
		5885		ARG	744	40.484 5.153 35 106 1
	rom !	5886		ARG	744	48.849 4.343 34 027 3 27
	OM !	5887		ARG		49.326 5.224 32 860 3
	'OM	888			744	40.322 6.200 32 324
	OM 5	889			744	48.944 7.100 31 362 7 7
TA		891	-	_	744	48.050 8.203 30 361 1.00 28.55
AT	OM 5	892	NH1 A	D. C.	744	48.429 9.409 30 547 1 00
AT(	OM 5	895	NH2 A		744	49.707 9.700 30.357
ATO	OM 5	898		D.C.	744	47.516 10.354 30.386
ATC	OM 5	899			44	50.016 3.454 34.452
ATC		900			44	50.794
ATO		901			45	50.133 2.251
ATO		902			4.5	49.248 1 500 - 33.869 1 00 46.36
ATO		03		. ~	45	51.261 1.402 52.521 1.00 45.54
ATO					45	50.972 0.070 1.00 43.41
ATO					15	50.155 0.403 33.34/ 1.00 41.77
ATO	M 59			_ ′ ′	15	52.590 2.00% 32.354 1.00 42.26
ATON						52,621 2,005 25 1.00 40.30
ATOM	_					53.679 1 570 1.00 39.73
ATOM	1 59					54.997 2.056 32.433 1.00 39.14
ATOM				• •	6	55,992 3 704 34.039 1.00 38.35
ATOM	591				6	56.202 0 776 35.249 1.00 36.75
ATOM						55.477 3 000 33.769 1.00 32.25
MOTA			~~~~			55.568 1 100 10 30.31
ATOM	591					55.185 -0.000 1.00 37.90
ATOM	591					56.490 1 504 32.938 1.00 37.99
ATOM	591					57.106 0 716 1.00 35.94
ATOM	592			747		58.124 1.460 35.00
ATOM	592			747		57.512 2 124 30.309 1.00 30.45
ATOM	5922		O1 PHE	747		56.950 1.450 27.61
ATOM	5923	CE	2 PHE	747		57.468 2 555 20.103 1.00 23.68
ATOM	5924		1 PHE	747		56.352 2 200
ATOM	5925			747		56.869 4 300 27.033 1.00 23.56
ATOM	5926			747		56.312 3 470 26.92
ATOM	5927		PHE	747		57.766 -0 477 23 25 1.00 26.21
ATOM	5928	N	PHE	747		57,920 -1 535 31.626 1.00 36.37
MOTA	5930		LYS	748		58.177 -0.312 1.00 37.11
ATOM	5931	CA	LYS	748		58.797 1 433
ATOM	5932	CB	LYS	748		59.433 -0.805
ATOM	5933	CG	LYS	748		59 978 1 004 1.00 46.17
ATOM	5934	CD	LYS	748		60.794 1.400 54.78
ATOM	5935	CE	LYS	748		61.239 -2.525 37.135 1.00 58.53
ATOM	5939	NZ	LYS	748		62 167 2 227 38.075 1.00 59.33
ATOM	5940	C	LYS	748		57 723 -2 463 39.120 1.00 62.36
ATOM	5940	0	LYS	748		57,998 3 66: 34.111 1.00 42.78
ATOM		N	GLN	749		56 503 1 000 34.075 1.00 37.97
ATOM	5943	CA	GLN	749		55 365 2 34.392 1.00 43.27
	5944	CB	GLN	749		54 146 2 25
						54.146 -2.056 35.146 1.00 47.37

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ATOM	5945	CG	GLN	749	54.236	-1.504	36.569	1.00 51.86
MOTA	5946	CD	GLN	749	53.036	-0.639	36.938	1.00 54.76
ATOM	5947	OE1	GLN	749	53.181	0.504	37.350	1.00 58.36
ATOM	5948	NE2	GLN	749	51.846	-1.179	36.769	1.00 59.25
MOTA	5951	C	GLN	749	55.006	-3.607	33.389	1.00 41.66
ATOM	5952	0	GLN	749	54.978	-4.841	33.355	1.00 40.25
MOTA	5953	N	LEU	750	54.759	-2.843	32.327	1.00 41.47
MOTA	5955	CA	LEU	750	54.398	-3.387	31.018	1.00 40.00
ATOM	5956	CB	LEU	750	54.366	-2.279	29.966	1.00 40.55
MOTA	5957	CG	LEU	750	53.316	-1.174	30.112	1.00 39.94
ATOM	5958	CD1	LEU	750	53.714	0.019	29.257	1.00 41.03
MOTA	5959	CD2	LEU	750	51.952	-1.696	29.722	1.00 37.80
ATOM	5960	C	LEU	750	55.383	-4.452	30.581	1.00 39.61
MOTA	5961	0	LEU	750	54.990	-5.470	30.027	1.00 42.08
ATOM	5962	N	VAL	751	56.670	-4.207	30.804	1.00 40.63
ATOM	5964	CA	VAL	751	57.691	-5.177	30.422	1.00 39.65
ATOM	5965	СВ	VAL	751	59.115	-4.639	30.677	1.00 33.44
ATOM	5966	CG1	VAL	751	60.142	-5.694	30.351	1.00 31.57
ATOM	5967	CG2	VAL	751	59.372	-3.433	29.825	1.00 25.19
ATOM	5968	C	VAL	751	57.458	-6.468	31.204	1.00 43.58
ATOM	5969	0	VAL	751	57.530	-7.563	30.646	1.00 44.81
ATOM	5970	N	GLU	752	57.116	6.339	32.481	1.00 46.24
ATOM	5972	CA	GLU	752	56.869	-7.518	33.301	1.00 50.55
MOTA	5973	СВ	GLU	752	56.781	-7.137	34.783	1.00 53.70
ATOM	5974	CG	GLU	752	58.090	-6.541	35.310	1.00 56.60
ATOM	5975	CD	GLU	752	58.079	-6.243	36.792	1.00 56.20
ATOM	5976		GLU	752	58.387	-5.092	37.178	1.00 53.45
ATOM	5977		GLU	752	57.789	-7.170	37.573	1.00 60.28
ATOM	5978	C	GLU	752	55.622	-8.275	32.837	1.00 50.90
ATOM	5979	ō	GLU	752	55.689	-9.474	32.555	1.00 50.50
ATOM	5980	N	ASP	753	54.501	-7.570	32.708	1.00 51.12
ATOM	5982	CA	ASP	753	53.251	-8.184	32.265	1.00 48.76
ATOM	5983	CB	ASP	753	52.122	-7.160	32.249	1.00 51.11
ATOM	5984	CG	ASP	753	51.646	-6.805	33.636	1.00 54.97
ATOM	5985		ASP	753	51.592	-7.715	34.495	1.00 54.37
ATOM	5986	OD2	ASP	753	51.319	-5.618	33.864	1.00 56.38
ATOM	5987	C	ASP	753	53.381	-8.790	30.881	1.00 48.02
ATOM	5988	0	ASP	753	52.991	-9.935	30.672	1.00 48.32
ATOM	5989	N	LEU	754	53.925	-8.020	29.940	1.00 45.16
ATOM	5991	CA	LEU	754	54.111	-8.490	28.571	1.00 44.82
ATOM	5992	CB	LEU	754	54.696	-7.387	27.691	1.00 42.70
ATOM	5993	CG	LEU	754	53.736	-6.263		
ATOM	5994	CD1		754	54.500		27.298	1.00 42.92
ATOM	5995	CD2		754	52.537	-5.236	26.495	1.00 41.44
ATOM	5996	C				-6.822	26.502	1.00 42.86
ATOM	5997	0	LEU LEU	754 754	55.001	-9.716 -10.606	28.529	1.00 46.00
ATOM	5998	N				-10.606	27.708	1.00 45.88
			ASP	755 766	55.975	-9.752	29.424	1.00 47.37
ATOM	6000	CA	ASP	755		-10.873	29.516	1.00 48.88
ATOM	6001	CB	ASP	755 755		-10.584	30.628	1.00 49.89
ATOM	6002	CG	ASP	755		-11.616	30.717	1.00 51.73
ATOM	6003	OD1		755		-11.680	31.785	1.00 55.47
ATOM	6004	OD2	ASP	755	59.236	-12.354	29.738	1.00 50.98

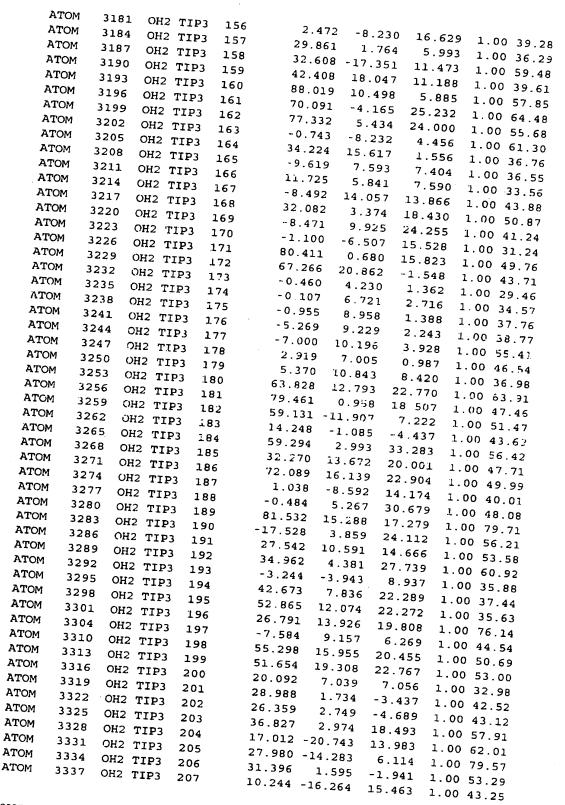


А	TOM 600	_		
	<b>—</b>	_	ASP 755	56.024 -12.093 29.864 1 00.51
			ASP 755	56 001 - 1-0 1-0 1 26
	T00,		ARG 756	55 227 "- 29.155 1.00 50 49
	70		ARG 756	54 332 37 30.917 1.00 52 15
			ARG 756	53 556 15 31.385 1.00 53 30
		CG	ARG 756	52 300 12 32.611 1.00 54.54
		CD .	ARG 756	+3.300 31 020 7 20 -
	OM 6013	NE	ARG 756	2.//2 34 215 3 00 -
	OM 6015	CZ i	ARG 756	51.293 -11.382 33 969 3
AT		NH1 A	ARG 756	30.259 -11.002 33 331
AT		NH2 A	ARG 756	49.487 -11.909 32.642
ATO			RG 756	49.9869.711 33.064
ÄTC		_	RG 756	33.35/ -13.420 30 207
ATC	OM 6024			53.243 -14.607 30.000 1.55.03
ATC				52.687 -12.452 29.680 1 34.82
ATO			,	51.709 -12 722
ATO	M 6028	CG2 II		51.025 -11 425
ATO	M 6029	CG1 II		50.112 -11 750 0 - 1.00 47.88
ATO	M 6030		_	50.247 -10 763
ATO		_		49.651
ATOM	V C035			52.314 -13.400
ATOM	4	O II		51.694 114 400 1.00 48.30
ATOM	1	N VA		53,523 -13 004 3.50 45.61
ATOM	1	CA VA		54 202 -13 734 7- 100 48 88
ATOM		CB VA	L 758	55,602 -13 701 67 1.00 49.96
ATOM		CG1 VA		56 212 25.615 1.00 47 80
ATOM		CG2 VAI	, .	55 461 " 24.502 1.00 44.17
ATOM	6045	****	758	54 370 25.188 1.00 46 65
ATOM		***	758	54 212 25.21/ 25.196 1.00 54 00
ATOM	2047 1/		759	54 607 25.306 1.00 53 52
ATOM		A ALA	759.	54 800 45 27.445 1.00 57 83
ATOM		B ALA	759	55 447 1.00 61 94
ATOM	6045 C		759	53 500 29.257 1.00 62.30
ATOM	6046 O	ALA	759	53 555 27.761 1.00 65 09
ATOM	6047 N	LEU	760	52 510 27.254 1.00 66 39
ATOM	6049 C	A LEU	760	51 300 17
ATOM	6.050 CE	3 LEU	760	1.14U JR DAE 11 65
ATOM	6051 CG		760	
ATOM	6052 CD	1 LEU	760	~~ . +1.330 (0 779 ,
	6053 CD	2 LEU	760	+4.303 (1 722 )
ATOM	6054 C	LEU	760	+0.019 {1 No
ATOM	6055 O	LEU	760	· - · - · · · · · · · · · · · · · · · ·
ATOM	6056 N	THR	761	49.342 -18.039 26 707
ATOM	6058 CA	THR	761	31.210 -17.201 25 860 1
ATOM	6059 CB	THR	761	30.626 -17.113 24 510
ATOM	6060 OG1			50.963 -15.760 23 R20 3 - 75.72
ATOM	6062 CG2		761 763	50.353 -14.690 24 555
ATOM	6063 C	THR	761 761	50.435 ~15.731 22 420 1 4.44
ATOM	6064 O	THR	761 763	51.080 -18.276 23 636 1 00 70.32
ATOM	6065 SG		761	52.276 -18.520 23.463 1.00 /4.66
ATOM	6066 CG		1603	19.100 0 000
ATOM	6067 SD	MET	534	69.385 12.295 23.303 0.50 30.84 PRT2
3	CO	MET	534	69.112 13.312 24.833 0.50 33.69 PRT2
	P068 CE	MET	534	70 067 12 400 24.032 0.50 34.44 PRT2
				70.067 12.429 26.060 0.50 36.92 PRT2

ATOM	6069	SG CY	S 603	56.370	-7.959	16.451	0.50	41.20	PRT2
ATOM	2716	OH2 TI	P3 1	71.864	25.128	2.721	1.00	26.20	
MOTA	2719	OH2 TI	P3 2	39.862	4.160	16.115	1.00	42.43	
ATOM	2722	OH2 TI	P3 3	83.875	19.969	10.572	1.00	23.41	
MOTA	2725	OH2 TI	P3 4	83.585	20.356	7.953	1.00	30.15	
ATOM	2728	OH2 TI	P3 5	75.100	16.407	6.948	1.00	46.78	
ATOM	2731	OH2 TI	P3 6	86.616	19.701	9.707	1.00	44.37	
ATOM	2734	OH2 TI			10.726	24.472		40.13	
ATOM	2737	OH2 TI	P3 8	55.346	9.394	22.489		29.09	
ATOM	2740	OH2 TI	P3 9	56.794	4.380	32.527		28.02	
ATOM	2743	OH2 TI	P3 10		4.653	13.421		18.63	
ATOM	2746	OH2 TI		41.527	5.347	22.682		32.60	
ATOM	2749	OH2 TI		44.868	9.058	21.659		34.90	
ATOM	2752	OH2 TI		64.548	-2.881	29.048		32.56	
ATOM	2755	OH2 TI		77.179	13.205	23.892		30.36	
ATOM	2758	OH2 TI		79.309	16.826	18.132		55.69	
ATOM	2761	OH2 TI		83.279	11.681	16.069		21.18	
MOTA	2764	OH2 TI		13.978	-9.614	0.374		23.81	
MOTA	2767	OH2 TI		38.294	0.616	5.237		48.89	
ATOM	2770	OH2 TI		27.114	6.248	5.051		19.82	
ATOM	2773	OH2 TI		34.369	-1.759			43.83	
ATOM	2776	OH2 TI		20.500	2.296	28.237		53.46	
ATOM	2779	OH2 TI			-11.733	38.257		51.73	
ATOM	2782	OH2 TI		17.066	-5.917	-2.027		29.88	
ATOM	2785	OH2 TI		27.873	8.078	15.136		45.40	
ATOM	2788	OH2 TI		31.459	0.037	6.873		33.38	
ATOM	2791	OH2 TI			-12.845	27.724		37.01	
ATOM	2794	OH2 TI			-17.329	12.884		37.31	
ATOM	2797	OH2 TI		88.863	14.111	8.054		41.25	
ATOM	2800	OH2 TI			-3.712	11.489		30.72	
MOTA	2803	OH2 TI		34.895	4.269	18.658		28.99	
MOTA	2806	OH2 TI		80.531	18.007	9.739		23.83	
ATOM	2809	OH2 TI	P3 32	5.519	3.787	10.628		20.39	
ATOM	2812	OH2 TI		-10.523	5.304	11.469		20.31	
ATOM	2815	OH2 TI		29.538	-8.848	20.187		43.26	
ATOM	2818	OH2 TI		5.866	3.469	13.367		21.16	
ATOM	2821	OH2 TI	P3 36	31.810	3.038	0.203	1.00	65.03	
ATOM	2824	OH2 TI	P3 37	19.879	2.087	-3.828		34.62	
MOTA	2827	OH2 TI	P3 38	61.882	2.577	32.790	1.00	43.01	
ATOM	2830	OH2 TI		21.062	-6.897	-4.255	1.00	26.18	
ATOM	2833	OH2 TI	P3 40	-15.562	8.847	22.744	1.00	40.33	
MOTA	2836	OH2 TI	P3 41	40.043	2.380	8.610		65.14	
ATOM	2839	OH2 TI	P3 42	19.176	11.322	0.332		33.04	
ATOM	2842	OH2 TI		67.221	8.965	17.535	1.00	14.78	
ATOM	2845	OH2 TI	P3 44	87.877	18.828	18.789	1.00	50.00	
MOTA	2848	OH2 TI		74.676	17.083	4.253		43.45	
MOTA	2851	OH2 TI		29.458	16.709	10.527		37.44	
ATOM	2854	OH2 TI		66.590	7.242	15.359		27.63	
ATOM	2857	OH2 TI		85.038	21.651	5.881		27.12	
ATOM	2860	OH2 TI		-4.762	3.091	3.313		13.83	
ATOM	2863	OH2 TI		19.509	4.951	5.063		33.74	
ATOM	2866	OH2 TI		34.833	5.465	24.635		32.77	
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ATOM 2865 OH2 TIP3 52 34.907 -17.187 13.739 1.00 39.47 ATOM 2870 OH2 TIP3 53 60.000 7.568 27.982 1.00 31.38 ATOM 2876 OH2 TIP3 55 65.218 12.161 25.430 1.00 40.22 ATOM 2881 OH2 TIP3 55 65.218 12.161 25.430 1.00 40.29 ATOM 2881 OH2 TIP3 56 68.597 6.912 16.955 1.00 45.39 ATOM 2880 OH2 TIP3 57 73.486 20.957 19.260 1.00 49.23 ATOM 2880 OH2 TIP3 57 73.486 20.957 19.260 1.00 49.23 ATOM 2890 OH2 TIP3 59 38.679 10.933 5.669 1.00 27.07 ATOM 2899 OH2 TIP3 60 29.817 -9.690 -1.649 1.00 44.28 ATOM 2999 OH2 TIP3 61 49.332 1.501 12.262 1.00 37.60 ATOM 2902 OH2 TIP3 62 41.366 3.969 28.884 1.00 37.60 ATOM 2902 OH2 TIP3 65 30.278 18.435 13.217 1.00 48.75 ATOM 2914 OH2 TIP3 66 81.15 4.304 3.317 1.00 48.75 ATOM 2914 OH2 TIP3 66 81.15 4.304 3.317 1.00 48.75 ATOM 2920 OH2 TIP3 66 81.15 4.304 3.317 1.00 48.75 ATOM 2920 OH2 TIP3 67 73.460 18.707 22.744 1.00 37.60 ATOM 2920 OH2 TIP3 67 73.460 18.707 22.744 1.00 37.60 ATOM 2923 OH2 TIP3 69 6.8041 3.332 24.939 1.00 44.98 ATOM 2920 OH2 TIP3 70 66.672 4.643 28.739 1.00 42.39 ATOM 2923 OH2 TIP3 70 66.676 13.158 -1.023 1.00 42.78 ATOM 2923 OH2 TIP3 70 66.676 13.158 -1.023 1.00 42.78 ATOM 2935 OH2 TIP3 71 59.587 6.482 5.018 1.00 37.78 ATOM 2935 OH2 TIP3 73 65.676 13.158 -1.023 1.00 42.78 ATOM 2935 OH2 TIP3 74 ATOM 2935 OH2 TIP3 75 0.3346 4.795 1.00 40.93 1.00 42.79 ATOM 2935 OH2 TIP3 78 68 6.566 13.158 -1.023 1.00 42.74 ATOM 2935 OH2 TIP3 78 69 6.666 6.378 9.673 1.00 10.0 12.98 ATOM 2935 OH2 TIP3 78 69 6.666 6.378 9.673 1.00 12.0 12.79 ATOM 2935 OH2 TIP3 78 69 6.666 6.378 9.673 1.00 12.00 12.79 ATOM 2935 OH2 TIP3 78 6.666 6.378 9.673 1.00 12.00 12.79 ATOM 2935 OH2 TIP3 78 6.666 6.378 9.673 1.00 12.00 12.79 ATOM 2940 OH2 TIP3 80 6.366 1.00 12.00 12.00 12.00 12.00 12.00 12.00 12.00 12.00 12.00 12.00 12.00 12.00 12.00 12.00 12.00 12.00 12.00 12.00 12.00 12.00 12.00 12.00 12.00 12.00 12.00 12.00 12.00 12.00 12.00 12.00 12.00 12.00 12.00 12.00 12.00 12.00 12.00 12.00 12.00 12.00 12.00 12.00 12.00 12.00 12.00 12.00 12.00 12.00 12.00 12.00 12.00 12.00 12.00 12.00 12.00 12.00 12.00 12.00 12.00 12.00 1	3 may :		
ATOM 2875 OH2 TIP3 54 60.000 7.568 27.982 1.00 39.47 ATOM 2878 OH2 TIP3 55 55.218 12.161 25.430 1.00 40.22 ATOM 2881 OH2 TIP3 55 55.218 12.161 25.430 1.00 40.22 ATOM 2881 OH2 TIP3 56 68.597 6.5912 16.955 1.00 45.39 ATOM 2889 OH2 TIP3 59 36.555 -8.367 -8.166 1.00 27.07 ATOM 2893 OH2 TIP3 60 29.817 -9.690 -1.649 1.00 44.28 ATOM 2899 OH2 TIP3 61 49.332 1.501 12.262 1.00 42.78 ATOM 2899 OH2 TIP3 62 41.366 3.969 28.834 1.00 37.60 ATOM 2990 OH2 TIP3 65 30.278 16.435 13.217 1.00 45.18 ATOM 2990 OH2 TIP3 65 30.278 16.435 13.217 1.00 45.18 ATOM 2911 OH2 TIP3 66 8.115 4.304 3.317 1.00 48.75 ATOM 2920 OH2 TIP3 66 8.115 4.304 3.317 1.00 48.75 ATOM 2920 OH2 TIP3 67 73.460 18.707 22.744 1.00 37.60 ATOM 2920 OH2 TIP3 68 -8.041 -3.332 24.939 1.00 44.78 ATOM 2920 OH2 TIP3 69 66.672 -4.643 28.739 1.00 44.78 ATOM 2920 OH2 TIP3 70 22.744 1.00 34.79 ATOM 2932 OH2 TIP3 70 22.744 1.00 34.79 ATOM 2933 OH2 TIP3 70 22.744 1.00 34.79 ATOM 2933 OH2 TIP3 70 22.744 1.00 34.79 ATOM 2935 OH2 TIP3 71 27.70 20.943 4.990 1.00 42.78 ATOM 2935 OH2 TIP3 71 27.70 20.943 4.990 1.00 42.78 ATOM 2935 OH2 TIP3 72 16.666 6.672 -4.643 28.739 1.00 42.74 ATOM 2935 OH2 TIP3 75 0.3314 2.779 50.999 1.00 42.78 ATOM 2935 OH2 TIP3 75 0.3314 2.779 50.999 1.00 42.78 ATOM 2935 OH2 TIP3 75 0.3314 2.779 50.999 1.00 42.78 ATOM 2941 OH2 TIP3 78 -8.546 6.378 9.673 1.00 17.89 ATOM 2950 OH2 TIP3 80 -8.546 6.388 9.673 1.00 17.89 ATOM 2950 OH2 TIP3 80 -8.546 6.388 9.673 1.00 17.89 ATOM 2968 OH2 TIP3 81 1.00 31.63 3.29 1.00 30.79 4.70 ATOM 2968 OH2 TIP3 82 20.319 3.556 1.00 39.55 2.73 ATOM 2968 OH2 TIP3 82 20.319 3.566 2.419 9.22 3.31 1.00 37.79 ATOM 2980 OH2 TIP3 80 4.476 1.2368 11.861 1.00 37.94 ATOM 2980 OH2 TIP3 80 4.476 1.2368 11.861 1.00 37.94 ATOM 2980 OH2 TIP3 80 4.476 1.2368 11.861 1.00 37.94 ATOM 2980 OH2 TIP3 80 4.476 1.2368 11.861 1.00 37.94 ATOM 2980 OH2 TIP3 80 4.476 1.2368 11.861 1.00 37.94 ATOM 2980 OH2 TIP3 80 4.476 1.2368 11.861 1.00 30.77 ATOM 2980 OH2 TIP3 99 4.476 4.476 1.2368 11.861 1.00 37.94 ATOM 2980 OH2 TIP3 99 4.476 4.476 1.2368 11.861 1.00 37.94 ATO		3 52	• • •
ATOM 2875 OH2 TIP3 54	ATOM 2872 OH2 TIP	_	34.307 ~17.187 13 730
ATOM 2881 OH2 TIP3 55 55.218 12.161 25.430 1.00 40.22 ATOM 2881 OH2 TIP3 56 68.597 6.912 16.955 1.00 45.39 ATOM 2883 OH2 TIP3 57 73.486 20.957 19.260 1.00 49.23 ATOM 2893 OH2 TIP3 58 35.55 -8.367 8.166 1.00 20.02 ATOM 2894 OH2 TIP3 60 38.079 10.933 5.669 1.00 27.07 ATOM 2896 OH2 TIP3 61 49.332 1.501 12.262 1.00 42.78 ATOM 2990 OH2 TIP3 62 41.366 3.969 28.834 1.00 37.60 ATOM 2990 OH2 TIP3 63 10.522 -13.468 0.864 1.00 37.60 ATOM 2990 OH2 TIP3 65 -1.001 -4.658 21.574 1.00 45.18 ATOM 2910 OH2 TIP3 66 8.115 4.304 3.171 1.00 46.04 ATOM 2910 OH2 TIP3 66 8.115 4.304 3.171 1.00 48.75 ATOM 2920 OH2 TIP3 66 8.115 4.304 3.171 1.00 44.28 ATOM 2920 OH2 TIP3 66 8.115 4.304 3.171 1.00 46.04 ATOM 2920 OH2 TIP3 68 -8.041 -3.332 24.939 1.00 44.96 ATOM 2920 OH2 TIP3 70 22.744 1.00 37.78 ATOM 2920 OH2 TIP3 70 22.744 1.00 37.78 ATOM 2920 OH2 TIP3 71 25.587 6.482 5.008 1.00 27.78 ATOM 2930 OH2 TIP3 70 2.770 2.993 4.990 1.00 62.39 ATOM 2931 OH2 TIP3 70 2.770 2.993 4.990 1.00 62.39 ATOM 2932 OH2 TIP3 71 25.587 6.482 5.008 1.00 37.78 ATOM 2935 OH2 TIP3 72 6.666 6.672 1.3.158 5.00 42.74 ATOM 2935 OH2 TIP3 78 75 0.334 27.795 10.999 1.00 31.20 ATOM 2941 OH2 TIP3 78 75 0.334 27.795 10.999 1.00 31.20 ATOM 2950 OH2 TIP3 78 78 7.975 10.999 1.00 31.20 ATOM 2950 OH2 TIP3 80 1.508 1.891 8.899 1.00 63.71 ATOM 2950 OH2 TIP3 80 1.508 1.891 8.899 1.00 37.78 ATOM 2950 OH2 TIP3 80 1.508 1.891 8.899 1.00 37.79 ATOM 2960 OH2 TIP3 80 1.508 1.891 8.899 1.00 37.94 ATOM 2980 OH2 TIP3 80 1.508 1.891 8.899 1.00 31.20 ATOM 2980 OH2 TIP3 80 1.508 1.891 8.899 1.00 31.20 ATOM 2980 OH2 TIP3 80 1.508 1.891 8.899 1.00 31.20 ATOM 2980 OH2 TIP3 80 1.508 1.508 1.891 1.891 1.00 37.79 ATOM 2980 OH2 TIP3 80 1.508 1.891 8.891 1.00 37.79 ATOM 2980 OH2 TIP3 80 1.508 1.508 1.00 37.79 ATOM 2980 OH2 TIP3 90 1.508 1.508 1.00 37.79 ATOM 2980 OH2 TIP3 91 1.508 1.508 1.00 37.99 ATOM 2980 OH2 TIP3 92 1.008 6.532 3.428 1.00 21.50 ATOM 2980 OH2 TIP3 93 1.008 6.532 3.428 1.00 20.39 ATOM 2980 OH2 TIP3 96 1.008 6.532 3.428 1.00 30.79 ATOM 2980 OH2 TIP3 96 1.008 6.508 1.008 37.99 ATOM 2980	2875 OH2 TER	_	60.000 7.568 27.992 4.00 39.47
ATOM 2884 OHZ TIP3 56 66.597 6.912 16.955 1.00 40.99 ATOM 2887 OHZ TIP3 57 73.486 20.957 19.260 1.00 45.39 ATOM 2890 OHZ TIP3 58 3.555 -8.367 -8.166 1.00 20.02 ATOM 2896 OHZ TIP3 60 29.817 -9.690 1.649 1.00 27.07 ATOM 2899 OHZ TIP3 61 49.332 1.501 12.262 1.00 42.78 ATOM 2900 OHZ TIP3 63 10.523 13.468 0.864 1.00 37.60 ATOM 2901 OHZ TIP3 65 30.278 16.455 13.217 1.00 16.04 ATOM 2905 OHZ TIP3 65 30.278 16.455 13.217 1.00 16.04 ATOM 2910 OHZ TIP3 66 30.278 16.455 13.217 1.00 16.04 ATOM 2911 OHZ TIP3 66 30.278 16.435 13.217 1.00 16.04 ATOM 2911 OHZ TIP3 66 8.8041 -3.332 24.939 1.00 44.78 ATOM 2920 OHZ TIP3 68 -8.041 -3.332 24.939 1.00 64.39 ATOM 2920 OHZ TIP3 70 66.672 -4.643 28.739 1.00 62.39 ATOM 2932 OHZ TIP3 71 59.587 6.482 5.018 1.00 37.78 ATOM 2932 OHZ TIP3 72 21.770 -20.943 4.990 1.00 62.39 ATOM 2932 OHZ TIP3 73 -15.177 7.529 4.524 1.00 19.90 ATOM 2933 OHZ TIP3 74 31.05 2.738 13.267 1.00 40.43 ATOM 2934 OHZ TIP3 75 78 78.786 6.378 9.673 1.00 17.89 ATOM 2947 OHZ TIP3 78 78 78.786 6.378 9.673 1.00 17.89 ATOM 2950 OHZ TIP3 80 1.508 7.389 6.309 1.00 37.78 ATOM 2950 OHZ TIP3 79 1.508 1.891 8.899 1.00 37.78 ATOM 2950 OHZ TIP3 80 1.508 7.399 1.00 37.78 ATOM 2950 OHZ TIP3 79 1.508 1.891 8.899 1.00 37.78 ATOM 2950 OHZ TIP3 79 1.508 1.891 8.899 1.00 37.78 ATOM 2950 OHZ TIP3 80 1.508 1.891 8.899 1.00 37.95 ATOM 2966 OHZ TIP3 80 1.508 1.891 8.899 1.00 37.95 ATOM 2966 OHZ TIP3 80 1.508 1.509 1.00 37.79 ATOM 2970 OHZ TIP3 80 1.508 1.891 8.891 1.00 17.89 ATOM 2980 OHZ TIP3 80 1.508 1.509 1.00 37.94 ATOM 2990 OHZ TIP3 80 1.508 1.509 1.00 37.94 ATOM 2990 OHZ TIP3 80 1.508 6.41 1.00 37.94 ATOM 2990 OHZ TIP3 80 1.508 6.41 1.00 37.94 ATOM 2990 OHZ TIP3 90 1.508 6.62 1.391 3.309 1.00 44.71 ATOM 2990 OHZ TIP3 80 1.508 6.41 1.00 37.94 ATOM 2990 OHZ TIP3 90 1.508 6.41 1.00 37.94 ATOM 2990 OHZ TIP3 91 1.508 6.41 1.00 37.94 ATOM 2990 OHZ TIP3 92 6.66 6.67 3.99 1.00 41.40 ATOM 2990 OHZ TIP3 93 44 1.00 37.94 ATOM 2990 OHZ TIP3 91 1.508 6.31 1.00 37.94 ATOM 2990 OHZ TIP3 92 6.69 1.508 1.508 1.00 37.94 ATOM 2990 OHZ TIP3 91 1.00 1.662 1.21	ATOM 2878 OH2 TID		-7.341 -1.418 6 300 1.00 31.38
ATOM 2887 OHZ TIP3 58	ATOM 2881 OH2 TID		55.218 12.161 25 430 1 25
ATOM 2887 OH2 TIP3 58 3.555 -8.367 -8.166 1.00 49.23 ATOM 2890 OH2 TIP3 59 38.079 19.266 1.00 49.23 ATOM 2890 OH2 TIP3 60 29.817 -9.690 -1.649 1.00 20.02 ATOM 2890 OH2 TIP3 61 49.332 1.501 12.262 1.00 42.78 ATOM 2890 OH2 TIP3 63 1.591 1.501 12.262 1.00 42.78 ATOM 2900 OH2 TIP3 63 1.052 -13.468 0.864 1.00 37.60 ATOM 2905 OH2 TIP3 64 -1.001 -4.658 21.574 1.00 37.60 ATOM 2910 OH2 TIP3 66 30.278 16.435 13.217 1.00 48.78 ATOM 2911 OH2 TIP3 66 30.278 16.435 13.217 1.00 48.78 ATOM 2911 OH2 TIP3 66 61.115 4.304 3.317 1.00 48.78 ATOM 2912 OH2 TIP3 66 61.115 4.304 3.317 1.00 48.78 ATOM 2910 OH2 TIP3 66 66.672 -4.632 28.744 1.00 34.79 ATOM 2920 OH2 TIP3 70 66.672 -4.632 28.799 1.00 42.78 ATOM 2920 OH2 TIP3 70 20.943 4.990 1.00 62.39 ATOM 2924 OH2 TIP3 71 59.587 6.482 5.018 1.00 37.78 ATOM 2932 OH2 TIP3 72 16.666 -13.158 -1.023 1.00 42.78 ATOM 2932 OH2 TIP3 73 -15.177 7.529 4.524 1.00 19.90 ATOM 2934 OH2 TIP3 75 0.334 -2.795 10.999 1.00 40.43 ATOM 2935 OH2 TIP3 75 0.334 -2.795 10.999 1.00 40.43 ATOM 2944 OH2 TIP3 76 0.334 -2.795 10.999 1.00 31.20 ATOM 2955 OH2 TIP3 78 -8.566 6.378 9.673 1.00 17.89 ATOM 2950 OH2 TIP3 78 -8.566 6.378 9.673 1.00 17.89 ATOM 2950 OH2 TIP3 80 0.366 -2.419 22.243 1.00 22.73 ATOM 2950 OH2 TIP3 81 0.366 -2.419 22.243 1.00 22.73 ATOM 2960 OH2 TIP3 85 10.581 -15.481 6.681 1.00 39.52 ATOM 2960 OH2 TIP3 85 10.581 -15.481 6.681 1.00 39.45 ATOM 2970 OH2 TIP3 85 10.581 -15.481 6.681 1.00 39.45 ATOM 2990 OH2 TIP3 85 10.581 -15.481 6.681 1.00 39.45 ATOM 2990 OH2 TIP3 86 1.362 3.916 4.424 1.00 37.94 ATOM 2990 OH2 TIP3 87 6.421 1.00 39.45 ATOM 2990 OH2 TIP3 99 1.0642 5.184 6.661 1.00 39.45 ATOM 2990 OH2 TIP3 99 1.0640 2.791 0.00 30.77 ATOM 2990 OH2 TIP3 99 1.0640 2.791 0.00 30.77 ATOM 2990 OH2 TIP3 99 1.0640 2.791 0.00 30.77 ATOM 2990 OH2 TIP3 99 1.0640 2.791 0.00 30.77 ATOM 2990 OH2 TIP3 99 1.00 4.791 0.00 30.77 ATOM 2990 OH2 TIP3 99 1.00 4.791 0.00 30.77 ATOM 2990 OH2 TIP3 99 1.00 4.791 0.00 30.77 ATOM 2990 OH2 TIP3 99 1.00 4.791 0.00 30.77 ATOM 2990 OH2 TIP3 99 1.00 4.791 0.00 30.77 ATOM 3001 OH2 TIP3 99 1	7.000		68.597 6 913 7 7 1.00 40.99
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ATOM 2914 OH2 TIP3 67 73.460 18.707 22.744 1.00 16.04 ATOM 2917 OH2 TIP3 68 -8.041 -3.332 24.939 1.00 42.79 ATOM 2923 OH2 TIP3 70 66.6.72 -4.643 28.739 1.00 42.98 ATOM 2929 OH2 TIP3 71 59.587 -6.482 5.018 1.00 37.78 ATOM 2932 OH2 TIP3 71 59.587 -6.482 5.018 1.00 37.78 ATOM 2932 OH2 TIP3 73 16.676 -13.158 -3.023 1.00 42.74 ATOM 2938 OH2 TIP3 74 33.105 2.738 13.267 1.00 40.43 ATOM 2938 OH2 TIP3 75 0.334 -2.795 10.999 1.00 31.20 ATOM 2941 OH2 TIP3 76 17.489 2.568 5.445 1.00 16.38 ATOM 2950 OH2 TIP3 77 27.373 3.870 6.168 1.00 16.38 ATOM 2955 OH2 TIP3 78 -8.546 6.378 9.673 1.00 17.89 ATOM 2955 OH2 TIP3 80 -4.985 -3.024 6.965 1.00 29.65 ATOM 2956 OH2 TIP3 82 20.339 3.536 4.985 -3.024 6.965 1.00 22.73 ATOM 2960 OH2 TIP3 82 20.339 3.536 1.00 22.73 ATOM 2960 OH2 TIP3 82 20.339 3.536 1.00 22.73 ATOM 2971 OH2 TIP3 85 10.581 -15.481 6.681 1.00 22.73 ATOM 2971 OH2 TIP3 86 4.476 -12.368 11.861 1.00 22.75 ATOM 2980 OH2 TIP3 87 ATOM 2980 OH2 TIP3 88 4.476 -12.368 11.861 1.00 22.15 ATOM 2980 OH2 TIP3 89 15.689 -7.291 -0.140 1.00 37.94 ATOM 2983 OH2 TIP3 90 -1.762 -5.389 3.937 1.00 27.79 ATOM 2980 OH2 TIP3 91 15.689 -7.291 -0.140 1.00 37.94 ATOM 2989 OH2 TIP3 92 46.342 -13.465 -0.010 1.00 37.94 ATOM 2980 OH2 TIP3 92 46.342 -13.465 -0.010 1.00 30.27 ATOM 2980 OH2 TIP3 93 ATOM 2980 OH2 TIP3 94 ATOM 2980 OH2 TIP3 95 10.408 5.632 3.428 1.00 20.37 ATOM 2980 OH2 TIP3 95 10.603 -7.291 -0.140 1.00 30.79 ATOM 2980 OH2 TIP3 97 73.207 -2.06 1.0677 1.00 30.04 7.94 ATOM 2999 OH2 TIP3 97 73.207 -2.06 1.0677 1.00 30.04 7.94 ATOM 2999 OH2 TIP3 99 34.6627 0.829 11.645 1.00 34.12 ATOM 3010 OH2 TIP3 99 36.627 0.829 11.645 1.00 34.12 ATOM 3010 OH2 TIP3 99 36.627 0.829 11.645 1.00 34.12 ATOM 3010 OH2 TIP3 99 36.627 0.829 11.645 1.00 31.03 ATOM 3010 OH2 TIP3 99 36.627 0.829 11.645 1.00 34.12 ATOM 3010 OH2 TIP3 99 36.627 0.829 11.645 1.00 34.12 ATOM 3010 OH2 TIP3 99 36.627 0.829 11.645 1.00 34.12 ATOM 3010 OH2 TIP3 99 36.627 0.829 11.645 1.00 34.12 ATOM 3010 OH2 TIP3 99 36.627 0.829 11.645 1.00 34.12 ATOM 3010 OH2 TIP3 99 36.627 0.829 11.645 1.00 34.1	2911 OH2 TIP3		30.2/8 16.435 13.217 1 00 40 75
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ATOM 2920 OH2 TIP3 69 ATOM 2923 OH2 TIP3 70 ATOM 2926 OH2 TIP3 71 ATOM 2929 OH2 TIP3 71 ATOM 2929 OH2 TIP3 71 ATOM 2932 OH2 TIP3 72 ATOM 2932 OH2 TIP3 73 ATOM 2932 OH2 TIP3 74 ATOM 2932 OH2 TIP3 74 ATOM 2938 OH2 TIP3 75 ATOM 2941 OH2 TIP3 76 ATOM 2944 OH2 TIP3 76 ATOM 2944 OH2 TIP3 77 ATOM 2950 OH2 TIP3 78 ATOM 2950 OH2 TIP3 78 ATOM 2950 OH2 TIP3 79 ATOM 2950 OH2 TIP3 78 ATOM 2950 OH2 TIP3 80 ATOM 2950 OH2 TIP3 80 ATOM 2950 OH2 TIP3 81 ATOM 2950 OH2 TIP3 82 ATOM 2950 OH2 TIP3 83 ATOM 2950 OH2 TIP3 84 ATOM 2950 OH2 TIP3 84 ATOM 2968 OH2 TIP3 85 ATOM 2968 OH2 TIP3 86 ATOM 2971 OH2 TIP3 87 ATOM 2972 OH2 TIP3 87 ATOM 2980 OH2 TIP3 87 ATOM 2974 OH2 TIP3 87 ATOM 2974 OH2 TIP3 87 ATOM 2975 OH2 TIP3 87 ATOM 2960 OH2 TIP3 87 ATOM 2960 OH2 TIP3 87 ATOM 2961 OH2 TIP3 86 ATOM 2970 OH2 TIP3 87 ATOM 2971 OH2 TIP3 86 ATOM 2971 OH2 TIP3 87 ATOM 2971 OH2 TIP3 87 ATOM 2972 OH2 TIP3 87 ATOM 2973 OH2 TIP3 87 ATOM 2974 OH2 TIP3 87 ATOM 2974 OH2 TIP3 87 ATOM 2975 OH2 TIP3 87 ATOM 2975 OH2 TIP3 87 ATOM 2970 OH2 TIP3 87 ATOM 2971 OH2 TIP3 86 ATOM 2971 OH2 TIP3 87 ATOM 2971 OH2 TIP3 87 ATOM 2972 OH2 TIP3 87 ATOM 2973 OH2 TIP3 87 ATOM 2974 OH2 TIP3 87 ATOM 2975 OH2 TIP3 87 ATOM 2970 OH2 TIP3 87 ATOM 2971 OH2 TIP3 87 ATOM 2971 OH2 TIP3 87 ATOM 2971 OH2 TIP3 87 ATOM 2970 OH2 TIP3 87 ATOM 2971 OH2 TIP3 87 ATOM 2972 OH2 TIP3 90 ATOM 2973 OH2 TIP3 91 ATOM 2974 OH2 TIP3 90 ATOM 2975 OH2 TIP3 91 ATOM 2980 OH2 TIP3 91 ATOM 2980 OH2 TIP3 92 ATOM 2980 OH2 TIP3 93 ATOM 2980 OH2 TIP3 94 ATOM 2980 OH2 TIP3 97 ATOM 3001 OH2 TIP3 98 ATOM 3001 OH2 TIP3 97	ATOM 2917 OH2 TIDE		73.460 18.707 22 744 2 2
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ATOM 2941 OH2 TIP3 75	7704	74	33.105 2 770 4.524 1.00 19.90
ATOM 2944 OH2 TIP3 76	ATOM	75	0.334 33 705
ATOM 2947 OH2 TIP3 78	ATOM -	76	17.489 2 560 1.00 31.20
ATOM 2950 OH2 TIF3 78	ATOM OILZ TIP3	77	27 272 2.300 3.445 1.00 16 38
ATOM 2953 OH2 TIP3 80	Amora	78	-8 546 6 5 6 1.00 39 52
ATOM 2956 OH2 TIP3 81 17.673 3.019 1.00 33.71 ATOM 2959 OH2 TIP3 82 20.319 3.536 2.883 1.00 22.73 ATOM 2965 OH2 TIP3 83 0.366 -2.419 22.243 1.00 22.15 ATOM 2968 OH2 TIP3 85 10.581 -5.481 6.681 1.00 13 22 ATOM 2971 OH2 TIP3 86 4.476 -12.368 11.861 1.00 43.14 ATOM 2977 OH2 TIP3 87 6.421 1.053 -3.368 11.00 21.50 ATOM 2980 OH2 TIP3 88 -13.766 1.683 5.565 1.00 39.45 ATOM 2980 OH2 TIP3 89 15.689 -7.291 -0.140 1.00 30.27 ATOM 2980 OH2 TIP3 90 -1.762 -5.389 3.937 1.00 31.03 ATOM 2990 OH2 TIP3 91 12.642 5.184 -4.424 1.00 37.94 ATOM 2990 OH2 TIP3 92 69.601 27.513 2.309 1.00 44.71 ATOM 2990 OH2 TIP3 94 60.354 -4.675 33.978 1.00 38.15 ATOM 3001 OH2 TIP3 95 10.408 5.632 3.428 1.00 51.37 ATOM 3000 OH2 TIP3 98 -3.042 5.487 30.579 1.00 30.78 ATOM 3010 OH2 TIP3 98 -3.042 5.487 30.579 1.00 30.78 ATOM 3010 OH2 TIP3 99 36.627 0.829 11.645 1.00 41.40 ATOM 3010 OH2 TIP3 99 36.627 0.829 11.645 1.00 41.40 ATOM 3010 OH2 TIP3 99 36.627 0.829 11.645 1.00 41.40 ATOM 3010 OH2 TIP3 99 36.627 0.829 11.645 1.00 41.40 ATOM 3010 OH2 TIP3 99 36.627 0.829 11.645 1.00 41.40 ATOM 3010 OH2 TIP3 99 36.627 0.829 11.645 1.00 41.40 ATOM 3010 OH2 TIP3 100 21.685 6.318 16.814 1.00 20.93 ATOM 3010 OH2 TIP3 101 31.434 0.662 19.231 1.00 57.99 ATOM 3020 OH2 TIP3 102 5.793 -8.713 22.177 1.00 55.61	ATTOM	79	1 500 9.673 1.00 17 89
ATOM 2959 OH2 TIP3 82 20.319 3.536 2.883 1.00 22.73 ATOM 2962 OH2 TIP3 83 0.366 -2.419 22.243 1.00 20.39 ATOM 2965 OH2 TIP3 84 19.688 -6.134 -1.678 1.00 13 22 ATOM 2971 OH2 TIP3 85 10.581 -15.481 6.681 1.00 43.14 ATOM 2974 OH2 TIP3 87 6.421 1.053 -3.368 1.00 21.50 ATOM 2977 OH2 TIP3 88 -13.766 1.683 5.565 1.00 39.45 ATOM 2980 OH2 TIP3 89 15.689 -7.291 -0.140 1.00 30.27 ATOM 2983 OH2 TIP3 90 -1.762 -5.389 3.937 1.00 31.03 ATOM 2989 OH2 TIP3 91 12.642 5.184 -4.424 1.00 37.94 ATOM 2995 OH2 TIP3 93 24.342 -13.465 -0.010 1.00 50.74 ATOM 2998 OH2 TIP3 94 60.354 -4.675 33.978 1.00 38.15 ATOM 3001 OH2 TIP3 96 -9.676 -3.916 4.621 1.00 34.12 ATOM 3004 OH2 TIP3 98 -3.042 5.487 30.579 1.00 30.78 ATOM 3010 OH2 TIP3 99 36.627 0.829 11.645 1.00 41.40 ATOM 3013 OH2 TIP3 99 36.627 0.829 11.645 1.00 30.78 ATOM 3019 OH2 TIP3 101 31.434 0.662 19.231 1.00 57.99 ATOM 3019 OH2 TIP3 102 5.793 -8.713 22.177 1.00 57.99 ATOM 3022 OH2 TIP3 103 -13.037 8.412 17.695 1.00 25.61	Amore Onz TIP3	80	2.071 8.809 7 OC 22 -
ATOM 2962 OH2 TIP3 82 20.319 3.536 2.883 1.00 20.39 ATOM 2965 OH2 TIP3 83 0.366 -2.419 22.243 1.00 20.39 ATOM 2968 OH2 TIP3 84 19.688 -6.134 -1.678 1.00 13 22 ATOM 2971 OH2 TIP3 85 10.581 -15.481 6.681 1.00 43.14 ATOM 2974 OH2 TIP3 87 6.421 1.053 -3.368 1.00 21.50 ATOM 2980 OH2 TIP3 89 15.689 -7.291 -0.140 1.00 30.27 ATOM 2983 OH2 TIP3 90 -1.762 -5.389 3.937 1.00 31.03 ATOM 2986 OH2 TIP3 91 12.642 5.184 -4.424 1.00 37.94 ATOM 2995 OH2 TIP3 93 24.342 -13.465 -0.010 1.00 50.74 ATOM 2998 OH2 TIP3 95 10.408 5.632 3.428 1.00 31.37 ATOM 2998 OH2 TIP3 95 10.408 5.632 3.428 1.00 38.15 ATOM 3001 OH2 TIP3 96 -9.676 -3.916 4.621 1.00 34.12 ATOM 3001 OH2 TIP3 98 -3.042 5.487 30.579 1.00 30.78 ATOM 3010 OH2 TIP3 99 36.627 0.829 11.645 1.00 41.40 ATOM 3016 OH2 TIP3 101 31.434 0.662 19.231 1.00 57.99 ATOM 3019 OH2 TIP3 102 5.793 -8.713 22.177 1.00 54.77 ATOM 3019 OH2 TIP3 102 5.793 -8.713 22.177 1.00 54.77 ATOM 3022 OH2 TIP3 103 -13.037 8.412 17.695 1.00 25.61	7 move	51	5 024 6.965 1 00 20 65
ATOM 2965 OH2 TIP3 83	ATOM OHZ TIP3		1./36 1 00 22 72
ATOM 2968 OH2 TIP3 84 19.688 -2.419 22.243 1.00 22.15  ATOM 2968 OH2 TIP3 85 10.581 -15.481 6.681 1.00 43.14  ATOM 2971 OH2 TIP3 86 4.476 -12.368 11.861 1.00 38.38  ATOM 2977 OH2 TIP3 88 -13.766 1.683 5.565 1.00 39.45  ATOM 2980 OH2 TIP3 89 15.689 -7.291 -0.140 1.00 30.27  ATOM 2983 OH2 TIP3 91 12.642 5.184 -4.424 1.00 37.94  ATOM 2989 OH2 TIP3 92 69.601 27.513 2.309 1.00 44.71  ATOM 2995 OH2 TIP3 93 24.342 -13.465 -0.010 1.00 50.74  ATOM 2998 OH2 TIP3 95 10.408 5.632 3.428 1.00 51.37  ATOM 3001 OH2 TIP3 96 -9.676 -3.916 4.621 1.00 34.12  ATOM 3010 OH2 TIP3 99 36.627 0.829 11.645 1.00 41.40  ATOM 3013 OH2 TIP3 100 21.685 6.318 16.814 1.00 20.93  ATOM 3019 OH2 TIP3 101 31.434 0.662 19.231 1.00 57.99  ATOM 3022 OH2 TIP3 102 5.793 -8.713 22.177 1.00 54.77  ATOM 3022 OH2 TIP3 103 -13.037 8.412 17.695 1.00 25.61	Amore Onz TIP3		2.883 1 00 20 22
ATOM 2968 OH2 TIP3 85	2965 OH2 TIP3		0.366 -2.419 22.243 1 00 33 15
ATOM 2971 OH2 TIP3 86 ATOM 2974 OH2 TIP3 87 ATOM 2977 OH2 TIP3 88 ATOM 2980 OH2 TIP3 89 ATOM 2983 OH2 TIP3 90 ATOM 2986 OH2 TIP3 91 ATOM 2989 OH2 TIP3 92 ATOM 2999 OH2 TIP3 93 ATOM 2995 OH2 TIP3 93 ATOM 2998 OH2 TIP3 94 ATOM 2998 OH2 TIP3 95 ATOM 2998 OH2 TIP3 95 ATOM 3001 OH2 TIP3 96 ATOM 3004 OH2 TIP3 97 ATOM 3004 OH2 TIP3 98 ATOM 3000 OH2 TIP3 99 ATOM 3010 OH2 TIP3 98 ATOM 3010 OH2 TIP3 99 ATOM 3011 OH2 TIP3 99 ATOM 3013 OH2 TIP3 99 ATOM 3016 OH2 TIP3 100 ATOM 3019 OH2 TIP3 101 ATOM 3019 OH2 TIP3 102 ATOM 3019 OH2 TIP3 102 ATOM 3022 OH2 TIP3 103 ATOM 3022 OH2 TIP3 100 ATOM 3019 OH2 TIP3 101 ATOM 3022 OH2 TIP3 102 ATOM 3022 OH2 TIP3 103 ATOM 3022 OH2 TIP3 103 ATOM 3022 OH2 TIP3 103 ATOM 3022 OH2 TIP3 100 ATOM 3022 OH2 TIP3 102 ATOM 3022 OH2 TIP3 103 ATOM 3022 OH2 TIP3 103 ATOM 3022 OH2 TIP3 103 ATOM 3022 OH2 TIP3 100 ATOM 3022 OH2 TIP3 100 ATOM 3022 OH2 TIP3 101 ATOM 3022 OH2 TIP3 102 ATOM 3022 OH2 TIP3 103 ATOM 3022 OH2 TIP3 103 ATOM 3022 OH2 TIP3 103 ATOM 3022 OH2 TIP3 100 ATOM 3022 OH2 TIP3 ATOM A 4.421 A.424 1.00	A10M 2968 OH2 TIP3		13.688 -6.134 -1.679
ATOM 2974 OH2 TIP3 87 6.421 1.053 -3.368 1.00 21.50  ATOM 2980 OH2 TIP3 88 -13.766 1.683 5.565 1.00 39.45  ATOM 2983 OH2 TIP3 90 15.689 -7.291 -0.140 1.00 30.27  ATOM 2986 OH2 TIP3 91 12.642 5.184 -4.424 1.00 37.94  ATOM 2992 OH2 TIP3 93 24.342 -13.465 -0.010 1.00 50.74  ATOM 2998 OH2 TIP3 95 10.408 5.632 3.428 1.00 51.37  ATOM 3001 OH2 TIP3 96 -9.676 -3.916 4.621 1.00 34.12  ATOM 3007 OH2 TIP3 98 -3.042 5.487 30.579 1.00 30.78  ATOM 3013 OH2 TIP3 99 36.627 0.829 11.645 1.00 41.40  ATOM 3016 OH2 TIP3 100 21.685 6.318 16.814 1.00 20.93  ATOM 3019 OH2 TIP3 101 31.434 0.662 19.231 1.00 57.99  ATOM 3019 OH2 TIP3 102 5.793 -8.713 22.177 1.00 54.77  ATOM 3022 OH2 TIP3 103 -13.037 8.412 17.695 1.00 25.61	A10M 2971 OH2 TID2		10.581 -15.481 6 691
ATOM 2980 OH2 TIP3 88 -13.766 1.683 5.565 1.00 21.50 ATOM 2983 OH2 TIP3 90 15.689 -7.291 -0.140 1.00 30.27 ATOM 2986 OH2 TIP3 91 12.642 5.184 -4.424 1.00 37.94 ATOM 2998 OH2 TIP3 92 69.601 27.513 2.309 1.00 44.71 ATOM 2995 OH2 TIP3 93 24.342 -13.465 -0.010 1.00 50.74 ATOM 2998 OH2 TIP3 95 10.408 5.632 3.428 1.00 51.37 ATOM 3001 OH2 TIP3 96 -9.676 -3.916 4.621 1.00 34.12 ATOM 3007 OH2 TIP3 98 -3.042 5.487 30.579 1.00 30.78 ATOM 3013 OH2 TIP3 99 36.627 0.829 11.645 1.00 41.40 ATOM 3016 OH2 TIP3 100 21.685 6.318 16.814 1.00 20.93 ATOM 3019 OH2 TIP3 102 5.793 -8.713 22.177 1.00 57.99 ATOM 3022 OH2 TIP3 103 -13.037 8.412 17.695 1.00 25.61	2974 OH2 TIP3		4.4/6 -12.368 11.861 1.00
ATOM 2980 OH2 TIP3 89	AIOM 2977 OH2 TIDE		0.421 1.053 -3.360
ATOM 2983 OH2 TIP3 90	2980 OH2 TITES		-13.766 1.683 5.565
ATOM 2986 OH2 TIP3 91 12.642 5.184 -4.424 1.00 37.94 ATOM 2999 OH2 TIP3 92 69.601 27.513 2.309 1.00 44.71 ATOM 2995 OH2 TIP3 94 60.354 -4.675 33.978 1.00 38.15 ATOM 3001 OH2 TIP3 96 -9.676 -3.916 4.621 1.00 34.12 ATOM 3007 OH2 TIP3 98 -3.042 5.487 30.579 1.00 30.78 ATOM 3010 OH2 TIP3 99 36.627 0.829 11.645 1.00 41.40 ATOM 3016 OH2 TIP3 100 21.685 6.318 16.814 1.00 20.93 ATOM 3019 OH2 TIP3 102 5.793 -8.713 22.177 1.00 57.99 ATOM 3022 OH2 TIP3 103 -13.037 8.412 17.695 1.00 25.61	ATOM 2983 OH2 TID2		15.689 -7.291 -0.140
ATOM 2989 OH2 TIP3 92 69.601 27.513 2.309 1.00 37.94  ATOM 2995 OH2 TIP3 93 24.342 -13.465 -0.010 1.00 50.74  ATOM 2998 OH2 TIP3 95 60.354 -4.675 33.978 1.00 38.15  ATOM 3001 OH2 TIP3 96 -9.676 -3.916 4.621 1.00 34.12  ATOM 3007 OH2 TIP3 98 -3.042 5.487 30.579 1.00 70.04  ATOM 3013 OH2 TIP3 99 36.627 0.829 11.645 1.00 30.78  ATOM 3016 OH2 TIP3 100 21.685 6.318 16.814 1.00 20.93  ATOM 3019 OH2 TIP3 102 5.793 -8.713 22.177 1.00 57.99  ATOM 3022 OH2 TIP3 103 -13.037 8.412 17.695 1.00 25.61	ATOM 2986 000		-1.762 -5.389 3 937
ATOM 2992 OH2 TIP3 93 ATOM 2995 OH2 TIP3 94 ATOM 2998 OH2 TIP3 95 ATOM 3001 OH2 TIP3 96 ATOM 3004 OH2 TIP3 97 ATOM 3007 OH2 TIP3 98 ATOM 3010 OH2 TIP3 99 ATOM 3013 OH2 TIP3 99 ATOM 3016 OH2 TIP3 100 ATOM 3016 OH2 TIP3 100 ATOM 3019 OH2 TIP3 101 ATOM 3020 OH2 TIP3 102 ATOM 3022 OH2 TIP3 103 ATOM 3022 OH2 TIP3 103 ATOM 3022 OH2 TIP3 103 ATOM 3037 OH2 TIP3 104 ATOM 304 OH2 TIP3 105 ATOM 305 OH2 TIP3 106 ATOM 306 OH2 TIP3 107 ATOM 307 OH2 TIP3 108 ATOM 308 OH2 TIP3 109 ATOM 309 OH2 TIP3 100 ATOM 3016 OH2 TIP3 101 ATOM 3019 OH2 TIP3 102 ATOM 3022 OH2 TIP3 103 ATOM 3022 OH2 TIP3 98 ATOM 3024 OH2 TIP3 98 ATO	ATOM 2989 OVA		12.642 5.184 -4 424
ATOM 2995 OH2 TIP3 94 60.354 -4.675 33.978 1.00 44.71 ATOM 2998 OH2 TIP3 95 10.408 5.632 3.428 1.00 51.37 ATOM 3001 OH2 TIP3 96 -9.676 -3.916 4.621 1.00 34.12 ATOM 3007 OH2 TIP3 98 -3.042 5.487 30.579 1.00 70.04 ATOM 3010 OH2 TIP3 99 36.627 0.829 11.645 1.00 41.40 ATOM 3016 OH2 TIP3 100 21.685 6.318 16.814 1.00 20.93 ATOM 3019 OH2 TIP3 102 5.793 -8.713 22.177 1.00 57.99 ATOM 3022 OH2 TIP3 103 -13.037 8.412 17.695 1.00 25.61	ATOM 2992 OVA		69.601 27.512 4.424 1.00 37.94
ATOM 2998 OH2 TIP3 95 10.408 5.632 33.978 1.00 38.15 ATOM 3001 OH2 TIP3 96 -9.676 -3.916 4.621 1.00 34.12 ATOM 3007 OH2 TIP3 98 -3.042 5.487 30.579 1.00 70.04 ATOM 3013 OH2 TIP3 100 21.685 6.318 16.814 1.00 20.93 ATOM 3019 OH2 TIP3 102 5.793 -8.713 22.177 1.00 57.99 ATOM 3022 OH2 TIP3 103 -13.037 8.412 17.695 1.00 25.61	ATOM 2995 OTTO TOTAL		24.342 -12 465 2.309 1.00 44.71
ATOM 3001 OH2 TIP3 96	7 TO 14	4	60.354 -4 675
ATOM 3004 OH2 TIP3 96	Amore CH2 TIP3 9	5	10.408 5 633
ATOM 3007 OH2 TIP3 97 73.207 -2.076 10.677 1.00 34.12  ATOM 3010 OH2 TIP3 98 -3.042 5.487 30.579 1.00 30.78  ATOM 3013 OH2 TIP3 100 21.685 6.318 16.814 1.00 20.93  ATOM 3019 OH2 TIP3 102 5.793 -8.713 22.177 1.00 54.77  ATOM 3022 OH2 TIP3 103 -13.037 8.412 17.695 1.00 25.61	The one of the state of the sta	6	3.428 1.00 51 37
ATOM 3010 OH2 TIP3 98 -3.042 5.487 30.579 1.00 70.04  ATOM 3013 OH2 TIP3 99 36.627 0.829 11.645 1.00 41.40  ATOM 3016 OH2 TIP3 101 21.685 6.318 16.814 1.00 20.93  ATOM 3019 OH2 TIP3 102 5.793 -8.713 22.177 1.00 57.99  ATOM 3022 OH2 TIP3 103 -13.037 8.412 17.695 1.00 25.61	Amov. 012 1113 9	7	72 202 4.621 1.00 34 12
ATOM 3013 OH2 TIP3 99 36.627 0.829 11.645 1.00 30.78  ATOM 3016 OH2 TIP3 100 21.685 6.318 16.814 1.00 20.93  ATOM 3019 OH2 TIP3 102 5.793 -8.713 22.177 1.00 54.77  ATOM 3022 OH2 TIP3 103 -13.037 8.412 17.695 1.00 25.61	Amore Onz TIP3 9	3	10.677 1.00 70 04
ATOM 3013 OH2 TIP3 100 21.685 6.318 16.814 1.00 41.40 ATOM 3016 OH2 TIP3 101 31.434 0.662 19.231 1.00 57.99 ATOM 3022 OH2 TIP3 103 -13.037 8.412 17.695 1.00 25.61	ATTOM 3010 OH2 TIP3 99	_	36.607 30.579 1.00 30 70
ATOM 3016 OH2 TIP3 101 31.434 0.662 19.231 1.00 20.93 ATOM 3019 OH2 TIP3 102 5.793 -8.713 22.177 1.00 54.77 ATOM 3022 OH2 TIP3 103 -13.037 8.412 17.695 1.00 25.61	ATOM 3013 OH2 TIP3 100		31.627 0.829 11.645 1.00 41 40
ATOM 3019 OH2 TIP3 102 5.793 -8.713 22.177 1.00 57.99 ATOM 3022 OH2 TIP3 103 -13.037 8.412 17.695 1.00 25.61	ATOM 3016 OH2 TIP3 101		21.685 6.318 16.814 1 00 20 20
ATOM 3022 OH2 TIP3 103 -13.037 8.412 17.695 1.00 25.61	3019 OH2 TIP3 103		0.662 19.231 1.00 57.00
8.412 17.695 1.00 25.61	MIUM 3022 Otto m		3./93 -8.713 22.177 1 00 54 77
1.00 25.61	103	-:	13.03/ 0.430
	\$\$\$D/\$\$145		25.61

ATOM	3025	OH2 TIP3	104	26.597	-10.647	-1.184	1.00 25.85
MOTA	3028	OH2 TIP3	105	24.406	1.951	18.037	1.00 30.72
ATOM	3031	OH2 TIP3	106	-1.809	12.914	3.754	1.00 43.57
ATOM	3034	OH2 TIP3	107	59.590	13.738	33.131	1.00 26.96
MOTA	3037	OH2 TIP3	108	4.442	-11.011	1.724	1.00 46.96
MOTA	3040	OH2 TIP3	109	8.101	2.869	0.801	1.00 37.28
MOTA	3043	OH2 TIP3	110	76.065	1.631	26.158	1.00 46.49
ATOM	3046	OH2 TIP3	111	48.821	15.839	14.239	1.00 34.18
ATOM	3049	OH2 TIP3	112	2.703	-11.324	8.959	1.00 39.16
MOTA	3052	OH2 TIP3	113	82.922	26.478	12.953	1.00 43.77
ATOM	3055	OH2 TIP3	114	8.998	-6.359	-3.309	1.00 39.51
ATOM	3058	OH2 TIP3	115	-8.590	4.563	4.397	1.00 32.53
ATOM	3061	OH2 TIP3	116	8.115	-13.800	8.351	1.00 41.64
MOTA	3064	OH2 TIP3	117	51.643	6.187	10.821	1.00 31.70
ATOM	3067	OH2 TIP3	118	20.737	3.915	15.522	1.00 17.40
ATOM	3070	OH2 TIP3	119	73.254	3.698	20.947	1.00 27.49
ATOM	3073	OH2 TIP3	120	5.343	-11.780	22.588	1.00 36.63
MOTA	3076	OH2 TIP3	121	34.390	2.307	16.660	1.00 64.04
ATOM	3079	OH2 TIP3	122	9.552	-11.846	6.934	1.00 28.23
ATOM	3082	OH2 TIP3	123	8.463	4.098	-1.454	1.00 30.21
MOTA	3085	OH2 TIP3	124	7.397	6.952	2.826	1.00 33.87
MOTA	3088	OH2 TIP3	125	35.796	-1.428	0.072	1.00 30.27
MOTA	3091	OH2 TIP3	126	45.044	10.052	11.102	1.00 28.75
ATOM	3094	OH2 TIP3	127	45.209	11.756	21.279	1.00 31.80
ATOM	3097	OH2 TIP3	128	-2.800	15.170	16.902	1.00 32.72
ATOM	3100	OH2 TIP3	129	85.885	11.248	9.428	1.00 25.28
ATOM	3103	OH2 TIP3	130	13.136	-2.420	1.867	1.00 20.56
ATOM	3106	OH2 TIP3	131	75.900	3.542	20.641	1.00 39.79
ATOM	3109	OH2 TIP3	132	13.075	7.580	-2.817	1.00 34.49
ATOM	3112	OH2 TIP3	133	11.166	-10.189	0.573	1.00 36.71
MOTA	3115	OH2 TIP3	134	13.814	-16.459	3.327	1.00 21.18
MOTA	3118	OH2 TIP3	135	-6.419	-3.460	16.599	1.00 32.62
ATOM	3121	OH2 TIP3	136	25.578	-12.834	3.624	1.00 43.32
MOTA	3124	OH2 TIP3	137	-16.472	11.136	6.388	1.00 64.77
MOTA	3127	OH2 TIP3	138	86.531	12.711	7.151	1.00 28.72
ATOM	3130	OH2 TIP3	139	32.292	-4.665	1.511	1.00 30.98
ATOM	3133	OH2 TIP3	140	45.116	7.369	11.774	1.00 30.59
ATOM	3136	OH2 TIP3	141	81.035	12.317	16.907	1.00 41.72
ATOM	3139	OH2 TIP3	142	2.905		-2.101	1.00 26.20
ATOM	3142	OH2 TIP3	143	31.895		20.885	1.00 36.12
ATOM	3145	OH2 TIP3	144		-2.640		1.00 58.90
MOTA	3148	OH2 TIP3	145		6.734	-1.116	1.00 37.81
ATOM	3151	OH2 TIP3	146		5.595	22.198	1.00 54.82
MOTA	3154	OH2 TIP3	147	68.337	-5.037	8.955	1.00 40.80
MOTA	3157	OH2 TIP3	148	0.191	-9.669	6.903	1.00 47.40
MOTA	3160	OH2 TIP3	149	68.043	18.153	10.710	1.00 36.67
MOTA	3163	OH2 TIP3	150	3.644	8.512	4.478	1.00 40.16
MOTA	3166	OH2 TIP3	151	52.117	11.302	18.644	1.00 40.22
MOTA	3169	OH2 TIP3	152	-10.220	6.750	4.981	1.00 25.00
MOTA	3172	OH2 TIP3	153	76.944	1.425	-0.793	1.00 46.95
MOTA	3175	OH2 TIP3	154		-11.958	17.014	1.00 38.99
ATOM	3178	OH2 TIP3	155	34.348	14.128	18.169	1.00 42.98





MOTA	3340	OH2	TIP3	208	7.255	-11.909	5.440	1.00	45.52
MOTA	3343	OH2	TIP3	209	-12.421	14.520	11.103	1.00	56.32
ATOM	3346	OH2	TIP3	210	11.250	9.879	-1.498	1.00	28.34
MOTA	3349	OH2	TIP3	211	11.426	12.574	-1.341	1.00	37.79
MOTA	3352	OH2	TIP3	212	34.344	13.104	-1.291	1.00	51.83
ATOM	3355	OH2	TIP3	213	31.230	18.082	8.054	1.00	44.77
MOTA	3358	OH2	TIP3	214	37.062	12.036	-1.875	1.00	53.61
MOTA	3361	OH2	TIP3	215	35.231	3.150	10.692	1.00	60.59
ATOM	3364	OH2	TIP3	216	63.913	13.371	26.770	1.00	59.44
ATOM	3367	OH2	TIP3	217	36.511	6.165	15.409		70.98
ATOM	3370	OH2	TIP3	218	90.623	4.459	6.671	1.00	52.23
ATOM	3373	OH2	TIP3	219	49.822	-11.758	10.881	1.00	46.12
ATOM	3376	OH2	TIP3	220	60.367	-10.286	16.662		68.41
ATOM	3379	OH2	TIP3	221	17.954	-21.378	7.048	1.00	68.51
ATOM	3382	OH2	TIP3	222	66.176	-1.266	30.784	1.00	39.19
MOTA	3385	OH2	TIP3	223	75.201	19.402	20.800	1.00	43.98
ATOM	3388	OH2	TIP3	224	-2.895	10.302	3.534		44.97
ATOM	3391	OH2	TIP3	225	6.045	-4.015	25.279	1.00	63.74
ATOM	3394	OH2	TIP3	226	36.238	5.898	12.819		32.89
ATOM	3397	OH2	TIP3	227	-5.516	16.713	14.089		51.60
ATOM	3400	OH2	TIP3	228	46.577	-11.931	26.964	1.00	37.76
ATOM	3403	ОН2	TIP3	229	6.496	6.048	13.722		27.51
MOTA	3406	OH2	TIP3	230	-3.691	-5.054	20.691	1.00	38.16
ATOM	3409	OH2	TIP3	231	1.811	-3.444	-0.149	1.00	
ATOM	3412	OH2	TIP3	232	86.148	11.480	23.402	1.50	57.66
MOTA	3415	OH2	TIP3	233	10.549	7.581	5.716	1.00	48.49
ATOM	3421	OH2	TIP3	234	64.680	-8.130	20.697	1 00	69.67
ATOM	3424	OH2	TIP3	235	11.380	-17.736	13.500	1.00	54.61
ATOM	3427	OH2	TIP3	236	3.136	-4.782	21.980	1.00	57.12
MOTA	3430	OH2	TIP3	237	72.296	1.006	-1.987	1.00	41.40
MOTA	3433	OH2	TIP3	238	50.258	-3.179	32.723	1.00	74.99
MOTA	3436	OH2	TIP3	239	58.051	9.469	11.776	1.00	44.10
ATOM	3439	OH2	TIP3	240	43.530	20.498	30.344	1.00	43.69
ATOM	3442	OH2	TIP3	241	67.081	16.597	15.934	1.00	45.80
ATOM	3445	OH2	TIP3	242	87.660	21.694	5.373	1.00	59.39
ATOM	3448	OH2	TIP3	243	71.779	28.586	1.932	1.00	61.12
ATOM	3451	OH2	TIP3	244	25.965	-8.124	27.084	1.00	42.13
ATOM	3454	OH2	TIP3	245	-18.336	10.487	12.859	1.00	73.36
MOTA	3457	OH2	TIP3	246	30.703	11.410	16.381	1.00	39.24
MOTA	3460	OH2	TIP3	247	22.617	-16.025	-2.906	1.00	63.22
ATOM	4620	С	SUG	1000	67.815	4.441	11.493	1.00	20.00
MOT'A	4621	C1	SUG	1000	67.387	3.706	10.364	1.00	20.00
ATOM	4622	И	SUG	1000	67.823	2.445	9.937	1.00	20.00
ATOM	4623	C2	SUG	1000	66.401	4.224	9.501	1.00	20.00
MOTA	4624	C3	SUG	1000	65.825	5.499	9.765	1.00	20.00
ATOM	4625	C4	SUG	1000	66.259	6.212	10.884	1.00	20.00
MOTA	4626	C5	SUG	1000	67.239	5.690	11.736	1.00	20.00
ATOM	4627	C6	SUG	1000	66.155	3.220	8.401		20.00
ATOM	4628	0	SUG	1000	67.372	1.047	8.275	1.00	20.00
MOTA	4629	C7	SUG	1000	67.155	2.121	8.828	1.00	20.00
ATOM	4630	C8	SUG	1000	63.369	2.460	5.852	1.00	
ATOM	4631	C9	SUG	1000	65.284	3.356	7.382		20.00





## TABLE 4

		y y Z OCC B
Atom	Atom A.A A.A	Λ
No.	туре туре №.	13.576 17.066 8.598 1.00 57.39
ATOM	1 N GEO 2-0-	12 446 17.198 7.684 1.00 33.03
ATOM	2 CA GEO	11 281 18.127 8.275 1.00 50.75
ATOM	3 CB GLU 1464 -	11 045 15.833 7.341 1.00 55.07
ATOM	4 C GLU 1464 "	13 722 15.504 6.165 1.00 59.72
ATOM	5 O GLU 1464	13 518 15.023 8.347 1.00 50.22
MOTA	6 N LEU 1465	9.087 1.00 44.20
ATOM	7 CA LEU 1465	-10.950 23.306 9 291 1.00 43.28
	8 CB LEU 1465	-10.133 13.716 9.227 1.00 43.70
ATOM	9 CG LEU 1465	9.013 1.00 47.59
MOTA	10 CD1 LEU 1465	-8.222 10.506 1.00 42.63
ATOM	11 CD2 LEU 1465	7 739 1.00 40.93
MOTA	12 C LEU 1465	-12.046 12.03
MOTA	13 O LEU 1465	-13.139 12.70
ATOM	14 N PRO 1466	5 844 1.00 39.07
MOTA	15 CD PRO 1466	-10.612 223 6 284 1.00 40.14
MOTA	16 CA PRO 1466	-12.754 10 10 4 981 1.00 40.90
MOTA	17 CB PRO 1466	5 202 1.00 41.39
MOTA	18 CG PRO 1466	7 305 1.00 40.06
MOTA	19 C PRO 1466	7 883 1.00 40.71
ATOM	770 1466	7 491 1.00 38.65
ATOM	20 0 07 17 1467	-14.064 9.175 8.467 1.00 39.24
MOTA	21 1 1467	-14.255 8.120 8.873 1.00 45.06
MOTA	22 CR CLU 1467	-15.722 8.034 5.00 50.91
MOTA	23 CE CIII 1467	-16.314 9.363 9.699 1.00 53.51
ATOM	~~ OTT 1467	-17.789 9.232 9.504 1.00 54.15
MOTA	25 05 777 1467	-18.379 8.170 1.00 53.10
MOTA	28 022 1467	-18.369 10.250 20.014 1.00 36.09
MOTA	27 GT 1 1467	-13.808 6.77
ATOM	28 5 5 1467	-13.922 6.523
MOTA	- ACD 1468	-13.272 5.929 0.407 1.00 28.23
MOTA	30 N 1468	-12.839 4.592 0.106 1 00 25.51
MOTA	31 CA 300 1468	-11.328 4.313 3.529 1.00 27.68
ATOM	ACD 1468	-10.885 3.207 7.572 1.00 26.01
MOTA	33 CO 1468	-11.623 2.133 6.962 1.00 28.87
ATOM	and ACD 1468	-9.777 3.107
ATOM	- an 1468	-13.274 3.027 1.00 25.83
MOTA	- ap 1468	-12.570 3.403 20.00 1.00 25.88
MOTA	nno 1469	-14.450 3.019 0.193 1.00 24.25
MOTA	36 N 200 1469	-15.396 3.173 100 26.69
ATOM	39 CD 2010	-14.963 2.079 20.641 1.00 28.81
MOTA	DDO 1469	-16.255 1.380 24.20
MOTA	41 CB DDO 1469	-16.702 2.770
ATOM	42 CG 200 1469	-14.012 0.923 20 0.0 27.60
MOTA	75 1469	-14.172 0.283 2230 1 00 26.49
MOTA	1470	-13.075 0.642 9.720 2.00
ATOM	45 1 1470	-12.108 -0.435 9.935 1.00 27.00
MOTA	46 CA ARG 1470	



Δ7	ГОМ									
		4	7 CB	ARG	1470					
	MO	4.8	CG	ARG	1470			-0.691	8.668	1 00 25 -
	'OM	49	CD	ARG	1470	<b>-2.</b>	073	-1.125	7.439	1.00 26.08
	MO	50	NE	ARG	1470	-11.	153	~1.257	6.213	1.00 30.77
AT		51	CZ	ARG		-10.	462	0.001	5.915	1.00 31.66
ATO		52		ARG	1470	<b>-</b> .9.;	577	0.167	4.941	1.00 30.94
ATO		53	NHO	ARG	1470	-9.2	249 .	0.846		1.00 33.30
ATO		54	C	ARG	1470	-8.9	990	1.346	4.144	1.00 32.78
ATC	M	55	ō		1470	~11.1		•	4.779	1.00 27.16
ATO	M	56	N	ARG	1470	-10.5			1.069	1.00 28.73
ATO	M	57	CA	TRP	1471	-10.8			1.673	1.00 27.30
ATO	M	58		TRP	1471	-9.8	_	_	1.363	1.00 27.98
ATO		59	CB	TRP	1471	-8.6		_	2.375	1.00 26.33
ATON	ч	50	CG	TRP	1471	-7.9		1.964 1	1.671	1.00 23.87
ATOM			CD2	TRP	1471	-7.11		0.947 10	7.795	1 00 24.61
ATOM		61		TRP	1471	-6.73		.104 11	205	1.00 23.32
ATOM		62	CE3	TRP :	1471	-6.58		0.807 10	.041	1.00 24.34
ATOM		63	CD1	TRP :	l471			.509 12	.438	1.00 21.39
ATOM		64	NE1	TRP ]	471	-8.12		.831 9		00 25.07
ATOM		65	CZ2		471	-7.36		.220 g		.00 26.82
ATOM			CZ3 7	TRP 1	471	-5.86		.898 10		00 23.12
ATOM		67	CH2 1		471	-5.72		.589 12		.00 21.02
			_		471	~5.364		265 11.		00 21.02
ATOM		€9 (	Т		471	-10.292		384 13.		.00 21.74
MOTA		10 V	ī G		172	- 9.551	2.	544 14.		.00 26.93
ATOM		71 C		_	172	-11.464	2.	975 13.	_	00 26.37
ATOM		72 C	_		72.	-11.909	3.	959 14.		00 26.40
ATOM		?3 c	_		72.	-13.168	4.	674 13.		00 27.12
ATOM		74 C				-13.497		026 14.4		00 28.25
ATOM			E1 GI		72	-12.611		180 14.0		OC 27.47
ATOM		76 OI	E2 GL			-11.877		39 13.0		00 24.64
ATOM	7	77 C	GL			-12.658	8.2			00 24.60
ATOM	7	8 0	GL			~12.179	3.4			00 23.70
.ATOM	7	9 N				-12.795	2.3			00 25.89
ATOM		0 CA	LE			-11.689	4.1		-	00 27.74
ATOM	8		,	,		-11.961	3.7		-	0 25.95
ATOM	8					-10.707	3.3			0 27.45
ATOM	8:					-10.958	3.09			0 24.99
ATOM	84		LEU			-11.55]	1.69		1.0	0 21.80
ATOM '	85		LEU			-9.646	3.19		1.0	0 20.63
ATOM	86		LEU			-12.478	5.00		1.00	0 22.34
ATOM	87	•	LEU		3	-12.007			2 1.00	29.33
ATOM	88		PRO	1474	<b>.</b>	-13.529	6.10		5 1.00	27.56
ATOM			PRO	1474	١.	-14.380	4.89		5 1.00	30.07
ATOM	89		PRO	1474		14.124	3.70		7 1.00	29.18
ATOM	90	CB	PRO	1474	_	15.266	6.05		7 1.00	29.03
ATOM	91	CG	PRO	1474		15.701	5.40		1.00	26.83
ATOM	92	C	PRO	1474		13.701	4.30	7 20.158	1.00	26.35
ATOM	93	0	PRO	1474	_		6.715	21.178	1.00	31.01
ATOM	94	N	ARG	1475	-		6.042	21.850		33.14
	95	CA	ARG	1475			8.038	21.178		31.33
ATOM	96		ARG	1475			8.810	21.973		31.33
ATOM	97		ARG	1475			0.292	21.791	1 00	32.99 35.87
MOTA	98		ARG	1475	-]		0.729	20.413	1 00	33.87
					-1	1.984 1	2.228	20.247	1.00 1.00	43.88
SSSD/5503	4 **	0.1							00	**.84

**ATOM** 99 NE ARG 1475 -11.665 12.499 18.846 1.00 48.59 MOTA 100 CZARG 1475 -10.435 12.663 18.374 1.00 46.00 ATOM 101 NH1 ARG 1475 -9.400 12.618 19.202 1.00 46.56 **ATOM** 102 NH2 ARG 1475 -10.241 12.746 17.065 1.00 44.18 MOTA 103 С ARG 1475 -12.175 8.456 23.442 1.00 35.47 **ATOM** 104 0 ARG 1475 -11.115 8.400 24.072 1.00 37.44 **ATOM** 105 ASP N 1476 -13.347 8.134 23.974 1.00 35.04 **ATOM** 106 CA ASP 1476 -13.468 7.800 25.380 1.00 34.30 MOTA 107 CB ASP 1476 -14.940 7.853 25.797 1.00 36.89 **ATOM** 108 CG ASP 1476 -15.796 6.818 25.089 1.00 38.67 **ATOM** 109 OD1 ASP 1476 -15.288 6.056 24.234 1.00 41.19 ATOM OD2 ASP 110 1476 -16.995 6.758 25.406 1.00 48.08 **ATOM** С ASP 111 1476 -12.858 6.457 25.770 1.00 33.67 ASP **ATOM** O 1476 112 -12.830 6.109 26.949 1.00 36.57 **ATOM** N ARG 113 1477 -12.441 5.670 24.781 1.00 32.72 MOTA 114 CA ARG 1477 -11.828 1.00 29.68 4.370 25.033 **ATOM** 115 CB ARG 1477 -12.117 3.418 23.886 1.00 25.53 **ATOM** ARG 116 CG 1477 -13.564 3.189 23.599 1.00 23.83 ATOM 117 ARG CD 1477 -14.234 2.525 24.772 1.00 26.80 MOTA 118 NE ARG 1477 -14.493 3.485 25.842 1.00 27.24 MOTA 119 CZARG 1477 -14.818 3.145 27.085 1.00 27.41 **ATOM** 120 NH1 ARG 1477 -14.931 1.874 27.438 1.00 29.00 **ATOM** 121 NH2 ARG 1477 -15.005 4:095 27.985 1.00 25.85 **ATOM** 122 C ARG 1477 -10.316 4.489 25.177 1.00 30.44 ATOM 123 0 ARG 1477 -9.616 3.515 25.461 1.00 32.78 MOTA 124 N LEU 1478 -9.800 5.690 25.002 1.00 30.39 **ATOM** 125 CA LEU 1478 -9.370 5.883 25.080 1 00 31.96 **ATOM** 126 CB LEU 1478 -7.886 6.508 23.771 1.00 30.43 MOTA 127 CG LEU 1478 -6.400 6.424 23.431 1.00 31.90 MOTA 128 CD1 LEU 1478 -5.939 4.964 23.382 1.00 28.92 MOTA 129 CD2 LEU 1478 -6.159 7.115 22.102 1.00 33.55 **ATOM** 130 C LEU 1478 -7.974 6.757 26.265 1.00 33.60 MOTA 131 0 LEU 1478 -8.193 7.972 26.251 1.00 33.96 MOTA VAL 132 N 1479 -7.416 6.140 27.305 1.00 33.54 **ATOM** 133 CA VAL 1479 -6.974 6.902 28.468 1.00 32.52 ATOM 134 CB VAL 1479 ~7.085 6.089 29.757 1.00 32.76 MOTA 135 CG1 VAL 1479 -6.728 6.973 30.926 1.00 33.27 MOTA 136 CG2 VAL 1479 -8.493 5.537 29.913 1.00 30.15 **ATOM** 137 C VAL 1479 -5.529 7.341 28.239 1.00 34.24 ATOM 138 0 VAL 1479 -4.581 6.546 28.350 1.00 32.24 ATOM 139 N LEU 1480 -5.381 8.607 27.867 1.00 35.88 MOTA 140 CA LEU 1480 -4.077 9.192 27.569 1.00 38.43 **ATOM** 141 CB LEU 1480 -4.24110.541 26.855 1.00 36.93 ATOM 142 CG LEU 1480 -4.828 10.535 25.435 1.00 35.67 **ATOM** 143 CD1 LEU 1480 24.907 -4.762 11.952 1.00 32.47 ATOM 144 CD2 LEU 1480 -4.037 9.613 24.499 1.00 33.60 ATOM 145 C LEU 1480 -3.144 9.324 28.768 1.00 39.70 **ATOM** 146 0 LEU 1480 -3.511 9.912 29.784 1.00 39.88 **ATOM** 147 N GLY 1481 -1.912 8.842 28.610 1.00 39.70 MOTA 148 CA GLY 1481 -0.960 8.896 29.700 1.00 41.31 ATOM 149 C GLY 1481 0.349 9.633 29.474 1.00 44.39 ATOM 150 GLY 0 1481 0.429 10.626 28.744 1.00 45.69

ħ mc			
ATC	+31 M	LYS 1482	1.389 9 122 20 22
ATO	CA	LYS 1482	2 722 30.124 1.00 44 73
ATO	-33 CB	LYS 1482	30.069 1.00 46.01
ATO		LYS 1482	31.023 1.00 51 20
ATO		LYS 1482	5.135 9.056 30.744 1 00 57 10
OTA	0	LYS 1482	5.878 7.826 31.248 1.00 60 81
ATOM		LYS 1482	5.430 6.567 30.515 1 00 5
ATOM	1 158 C		6.235 5.375 30.912 1.00 5
ATOM		<del>-</del>	3.370 9.782 28.681 1 00 44
ATOM	1 160 N		3 440 9 700 1.00 46.09
ATOM	161 CD		3.886 10.969 28 324 1 02
ATOM		PRO 1483	3.910 12.704
ATOM	163 CB	PRO 1483	4.536 11 222 - 1.00 46.11
ATOM		PRO 1483	5.015 13.660 036 1.00 45.96
ATOM	165	PRO 1483	4.041 12 273
ATOM	266	PRO 1483	5.739 10 272 1.00 45.37
ATOM	165	PRO 1483	6.506 10 130 25 1.00 46.43
ATOM	100	LEU 1484	5 844 9 570
ATOM		LEU 1484	6.978 9.504
ATOM		LEU 1484	6.543 7.436 25.554 1.00 50.46
ATOM		EU 1484	5 655 24 811 1.00 49 38
ATOM	171 CD1 I	EU 1484	5 007 - 25.576 1.00 50.15
ATOM	172 CD2 I	EU 1484	5.422 24.615 1.00 44 90
ATOM		EU 1484	26.669 1.00 44 60
ATOM		EU 1484	24.764 1.00 53 33
		LY 1485	7 643 24.896 1.00 51 94
ATOM		LY 1485	9 603 23 23 931 1.00 57.68
ATOM		LY 1485	7 207 11.140 23.148 1.00 60.27
ATOM	178 () G	LY 1485	6 774 22.016 1.00 62.66
ATOM	179 N G	LN 1491	12.590 21.924 1 00 64 01
ATOM	180 C'A GI	N 1491	13.904 1 00 47 06
ATOM	181 CB GI		20.206 1 00 44 42
ATOM	182 C GL		3.3/3 14.829 20.918 1 00 44 31
ATOM	183 O GI	N 1491	3.755 12.433 20.170 1.00 43.00
ATOM	184 N VA	_	2.807 12.150 19.426 1 00 43 67
ATOM	185 CA VA		4.338 11.542 20.974 1 00 40 40
ATOM	186 CB VA		3.903 10.143 21 101 1 20 1
ATOM	187 CG1 VA		4.962 9.119 20.673
ATOM	188 CG2 VA	L 1492	4.416 7.721 20 897 1 00 -
ATOM	189 C VA		5.336 9.296 19 233 1 00 1
ATOM	190 O VAI		3.720 9.905 22.586 1 00 40 00
ATOM	191 N VAL		4.679 10.038 23 355 1.00 40.23
ATOM	192 CA VAL		2.516 9.518 22.993 1.00 22
ATOM	193 CB VAL		2.250 9.291 24.405 1.00 35.15
ATOM	194 CG1 VAL		1.131 10.245 24 924 1 00
ATOM		_	1.386 11.656 24 422 1 00 37.83
ATOM	*****	_	-0.252 9.769 24 508 1 00 36.45
ATOM		· · · · <del>-</del>	1 854 7 24.308 1.00 39.28
ATOM			1 450 7 330
3.770	100	1494	2 052 2 420 23.797 1.00 37.17
· ·	199 CA LEU	1494	1.645 6.00
3 mars	200 CB LEU	1494	2 445 5 500 20.335 1.00 30.87
3.000.	201 CG LEU	1494	1 970 4 252
	202 CD1 LEU	1494	2 124 2 220 20.141 1.00 28.67
			2.124 3.132 27.129 1.00 27.40

ATOM	203	CD2	LEU	1494	2.736	3.904	29.377	1.00 28.84
ATOM	204	С	LEU	1494	0.173	6.256	26.701	1.00 31.18
ATOM	205	0	LEU	1494	-0.249	7.344	27.119	1.00 30.88
ATOM	206	N	ALA	1495	-0 626	5.223	26.477	1.00 30.40
ATOM	207	CA	ALA	1495	-2.044	5.307	26.817	1.00 28.30
ATOM	208	CB	ALA	1495	-2.815	5.999	25.691	1.00 27.35
ATOM	209	C	ALA	1495	-2.608	3.919	27.057	1.00 26.32
ATOM	210	0	ALA	1495	-1.926	2.915	26.846	1.00 24.54
ATOM	211	N	GLU	1496	-3.836	3.867	27.552	1.00 28.11
ATOM	212	CA	GLU	1496	-4.51.4	2.603	27.793	1.00 29.22
MOTA	21.3	CB	GLU	1496	-4.841	2.441	29.272	1.00 31.77
ATOM	214	CG	GLU	1496	-3.627	2.233	30.140	1.00 37.26
ATOM	215	CD	GLU	1496	-3.950	2.405	31.613	1.00 39.77
ATOM	216	OE1	GLU	1496	-4.322	3.534	31.999	1.00 37.54
ATOM	217	OE2		1496	-3.835	1.417	32.378	1.00 41.52
ATOM	218	С	GLU	1496	-5.799	2.594	26.970	1.00 29 76
ATOM	219	9	GLU	1496	-6.593	3.543	27.020	1.00 31.39
ATOM	220	N	ALA	1497	-5.961	1.561	26.153	1.00 29.55
ATOM	221	CA	ALA	1497	-7.139	1.426	25.324	1.00 28.69
ATOM	222	CB	ALA	1497	-6.742	0.969	23.930	1.00 23.86
ATOM	223	C	ALA	1497	-8.068	J.418	25.965	1.00 29.51
ATOM	224	O	ALA	1497	-7.657	-0.762	26.278	1.00 30.40
ATOM	225	N	ILE	1498	-9.313	0.823	26.201	1.00 31.33
ATOM	226	CA	LLE	1498	-10.302	.0.064	26.811	1.00 32.30
ATOM	227	CB	ILE	1498	-11.359	0.727	27.619	1.00 33.61
ATOM	228	CG2	ILE	1498	-12.233	-0.246	28.439	1.00 34.55
ATOM	229	CG1	ILE	1498	-10.690	1.745	28.545	1.00 31.99
ATOM	230	CD1	ILE	1498	-11.663	2.730	29.155	1.00 26.68
MOTA	231	C	ILE	1498	-11.023	-0.777	25.673	1.00 32.69
ATOM	232	O	ILE	1498	-11 644	-0.134	24.838	1.00 32.03
ATOM	233	N	GLY	1499	-10.917	-2.095	25.610	1.00 37.34
ATOM	234	CA	GLY	1499	-11.588	-2.822	24.554	1.00 44.45
ATOM	235	C	GLY	1499	-10.709	-3.193	23.372	1.00 50.75
ATOM	236	O	GLY	1499	-9.993	-4.205	23.43B	1.00 53.68
ATOM	237	N	LEU	1500	-10.729	-2.370	22.321	1.00 51.14
ATOM	238	CA	LEU	1500	-9.963	-2.613	21.087	1.00 51.15
ATOM	239	CB	LEU	1500	-8.445	-2.677	21.345	1.00 50.85
ATOM	240	CG	LEU	1500	-7.516	-1.463	21.166	1.00 49.05
ATOM	241	CD1	LEU	1500	-6.082	-1.946	21.263	1.00 44.92
ATOM	242	CD2	LEU	1500	-7.703	-0.783	19.824	1.00 44.03
MOTA	243	С	LEU	1500	-10.420	-3.891	20.376	1.00 50.50
ATOM	244	0	LEU	1500	-10.544	-4.966	20.984	1.00 49.92
MOTA	245	N	PRO	1505	-13.321	-5.777	25.373	1.00 48.57
ATOM	246	CD	PRO	1505	-13.937	-7.111	25.286	1.00 50.09
ATOM	247	CA	PRO	1505	-14.289	-4.776	25.848	1.00 46.31
ATOM	248	CB	PRO	1505	-15.630	-5.503	25.710	1.00 45.25
ATOM	249	CG	PRO	1505	-15.271	-6.918	26.025	1.00 48.85
ATOM	250	C	PRO	1505	-14.010	-4.321	27.294	1.00 43.31
ATOM	251	0	PRO	1505	-14.001	-3.122	27.571	1.00 42.84
ATOM	252	N	ASN	1506	-13.712	-5.272	28.178	1.00 40.46
ATOM	253	CA	ASN	1506	-13.430	-4.945	29.571	1.00 42.33
ATOM	254	СВ	ASN	1506	-14.302	-5.776	30.512	1.00 43.55



ATOM 255 CG ASN 1506 -15.760 -5.436 30.382 1.00 42.68 ATOM 257 ND2 ASN 1506 -16.141 -4.269 30.316 1.00 47.11 ATOM 258 C ASN 1506 -16.591 -6.461 30.323 1.00 45.66 ATOM 259 O ASN 1506 -11.962 -5.097 29.597 10.00 42.89 ATOM 260 N ARG 1507 -11.617 -5.221 31.137 1.00 42.89 ATOM 261 CA ARG 1507 -9.661 -5.186 29.145 1.00 42.72 ATOM 262 CA ARG 1507 -9.661 -5.186 29.145 1.00 42.72 ATOM 263 CG ARG 1507 -9.407 -7.728 28.992 1.00 60.88 ATOM 264 C ARG 1507 -8.357 -8.063 30.38 1.00 50.39 ATOM 265 CZ ARG 1507 -8.357 -8.063 30.38 1.00 57.47 ATOM 266 CZ ARG 1507 -8.012 -9.861 31.691 1.00 74.19 ATOM 267 NH1 ARG 1507 -8.012 -9.861 31.691 1.00 74.19 ATOM 268 NH2 ARG 1507 -8.357 -8.063 30.38 1.00 60.88 ATOM 269 C ARG 1507 -8.318 -11.068 32.134 1.00 82.38 ATOM 270 O ARG 1507 -8.318 -11.068 32.134 1.00 82.38 ATOM 271 N VAL 1508 -7.927 33.491 29.279 1.00 35.19 ATOM 273 CB VAL 1508 -7.997 33.491 29.279 1.00 33.82 ATOM 274 CG1 VAL 1508 -7.997 33.491 29.279 1.00 33.82 ATOM 275 CG2 VAL 1508 -7.997 30.993 30.998 1.00 30.46 ATOM 276 C VAL 1508 -7.997 33.491 29.279 1.00 33.82 ATOM 278 N THR 1509 -5.427 -7.2152 27.154 1.00 31.02 ATOM 280 CB THR 1509 -5.427 -2.152 27.154 1.00 31.02 ATOM 280 CB THR 1509 -5.427 -2.152 27.154 1.00 31.02 ATOM 281 CG1 THR 1509 -5.427 -2.152 27.154 1.00 31.02 ATOM 282 CG2 THR 1509 -4.492 -3.101 26.493 1.00 82.97 ATOM 283 C THR 1509 -5.427 -2.152 27.154 1.00 31.02 ATOM 284 O THR 1509 -5.427 -2.152 27.154 1.00 31.02 ATOM 285 CG LYS 1510 -0.992 -0.595 27.648 1.00 30.47 ATOM 286 CB THR 1509 -4.492 -3.101 26.493 1.00 29.17 ATOM 286 CB THR 1509 -5.427 -2.152 27.154 1.00 31.02 ATOM 287 CG VAL 1511 -0.062 -2.352 -1.003 31.00 29.17 ATOM 288 CG LYS 1510 -0.992 -0.595 27.648 1.00 31.39 ATOM 280 CB THR 1509 -5.427 -2.152 27.154 1.00 31.02 ATOM 280 CB THR 1509 -6.426 -2.527 2.406 2.408 2.406 1.00 31.02 ATOM 280 CG THR 1509 -5.427 -2.152 27.154 1.00 31.02 ATOM 280 CG LYS 1510 -0.092 -0.595 27.648 1.00 31.00 29.17 ATOM 280 CG LYS 1510 -0.992 -0.595 27.648 1.00 30.10 ATOM 290 CD LYS 1510 -0.993 1.004 22.615 1.00 30.01 ATOM 290 CG V									
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ATOM 262 CB ARG 1507				_	-11.	0995			1.00 43.23
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ATOM 264 CD ARG 1507 -8.357 -8.063 30.038 1.00 60.88 ATOM 265 NE ARG 1507 -8.566 -9.401 30.574 1.00 74.19 ATOM 266 NIL ARG 1507 -8.066 -9.401 30.574 1.00 74.19 ATOM 267 NH1 ARG 1507 -8.012 -9.861 31.691 1.00 79.97 ATOM 268 NIL ARG 1507 -8.338 -11.068 32.134 1.00 82.38 ATOM 270 O ARG 1507 -8.338 -11.068 32.134 1.00 82.38 ATOM 271 N VAL 1508 -7.190 -2.335 28.782 1.00 38.15 ATOM 272 CA VAL 1508 -7.190 -2.335 28.782 1.00 33.82 ATOM 273 CB VAL 1508 -6.824 1.296 29.883 1.00 30.19 ATOM 274 CGI VAL 1508 -6.824 1.296 29.883 1.00 30.19 ATOM 275 CG2 VAL 1508 -6.824 1.296 29.883 1.00 30.19 ATOM 277 O VAL 1508 -5.948 -1.900 30.938 1.00 30.19 ATOM 278 N THR 1509 -8.002 -0.723 30.498 1.00 33.82 ATOM 279 CA THR 1509 -4.492 -3.916 28.555 1.00 33.91 ATOM 280 CB THR 1509 -4.492 -3.915 25.031 1.00 30.88 ATOM 281 CG THR 1509 -4.206 -2.527 26.476 1.00 30.88 ATOM 282 CG2 THR 1509 -3.325 26.481 1.00 30.88 ATOM 283 C THR 1509 -3.325 26.481 1.00 30.88 ATOM 284 O THR 1509 -3.325 26.496 1.00 33.90 ATOM 285 N LYS 1510 -0.117 -0.460 29.135 1.00 28.74 ATOM 286 CA LYS 1510 -0.914 1.065 -1.603 31.062 1.00 40.49 ATOM 289 CD LYS 1510 -0.117 -0.460 29.135 1.00 30.42 ATOM 290 CE LYS 1510 -0.813 -0.213 25.355 1.00 29.64 ATOM 291 NZ LYS 1510 -0.625 1.305 23.245 1.00 30.42 ATOM 292 C LYS 1510 -0.914 1.004 24.836 1.00 30.13 ATOM 296 CB VAL 1511 -0.904 1.004 24.836 1.00 30.13 ATOM 297 CG1 VAL 1511 -0.904 1.004 24.836 1.00 30.13 ATOM 298 CG LYS 1510 -0.625 1.305 23.245 1.00 30.42 ATOM 299 C VAL 1511 -0.904 1.004 24.836 1.00 30.13 ATOM 299 C VAL 1511 -0.904 1.004 24.836 1.00 30.13 ATOM 290 C VAL 1511 -0.904 1.004 24.836 1.00 30.13 ATOM 290 C LYS 1510 -0.625 1.305 23.245 1.00 30.93 ATOM 291 NZ LYS 1510 -0.625 1.305 23.245 1.00 30.42 ATOM 290 C LYS 1510 -0.625 1.305 23.245 1.00 30.42 ATOM 290 C LYS 1510 -0.625 1.305 23.245 1.00 30.93 ATOM 290 C LYS 1510 -0.904 1.004 24.836 1.00 30.13 ATOM 290 C LYS 1510 -0.904 1.004 24.836 1.00 31.09 ATOM 290 C LYS 1510 -0.904 1.004 24.836 1.00 30.13 ATOM 290 C LYS 1510 -0.904 1.004 24.836 1.00 30.13 ATOM 290 C LYS 1510 -0				,		44 -6			1.00 42.24
ATOM 266 C2 ARG 1507 -8.566 -9.401 30.574 1.00 74.19 ATOM 268 NH2 ARG 1507 -8.566 -9.401 30.574 1.00 74.19 ATOM 269 NH2 ARG 1507 -8.9861 31.691 1.00 79.97 ATOM 269 NH2 ARG 1507 -8.9861 31.691 1.00 79.97 ATOM 269 C ARG 1507 -8.9861 31.691 1.00 79.97 ATOM 270 O ARG 1507 -8.9861 32.134 1.00 82.38 ATOM 271 N VAL 1508 -7.937 3.491 29.279 1.00 36.46 ATOM 272 CA VAL 1508 -7.927 3.491 29.279 1.00 36.46 ATOM 273 CE VAL 1508 -7.927 3.491 29.279 1.00 33.19 ATOM 274 CG1 VAL 1508 -6.824 -1.296 29.883 1.00 30.19 ATOM 275 CG2 VAL 1508 -8.072 -0.723 30.498 1.00 33.82 ATOM 276 C VAL 1508 -6.824 -1.296 29.883 1.00 30.19 ATOM 277 O VAL 1508 -5.192 -2.869 28.155 1.00 33.91 ATOM 278 N THR 1509 -5.192 -2.869 28.155 1.00 33.91 ATOM 279 CA THR 1509 -5.192 -3.926 28.555 1.00 33.91 ATOM 280 CB THR 1509 -4.206 -2.527 26.476 1.00 30.47 ATOM 281 CG1 THR 1509 -4.206 -2.527 26.476 1.00 30.47 ATOM 282 CG2 THR 1509 -3.323 -1.300 24.491 ATOM 283 C THR 1509 -3.323 -1.300 24.491 ATOM 286 CA LYS 1510 -2.092 -1.432 26.883 1.00 29.17 ATOM 287 CB LYS 1510 -0.924 -0.219 26.039 1.00 27.29 ATOM 289 CD LYS 1510 -0.924 -0.219 26.039 1.00 29.17 ATOM 290 C LYS 1510 -0.924 -1.029 2.441 1.00 24.49 ATOM 290 C LYS 1510 -0.924 -1.029 2.325 2.45 1.00 31.32 ATOM 290 C LYS 1510 -0.924 -1.029 2.441 1.00 27.29 ATOM 291 NZ LYS 1510 -0.924 -1.029 2.245 1.00 30.10 ATOM 292 C LYS 1510 -0.924 -1.029 2.245 1.00 30.10 ATOM 293 O LYS 1510 -0.924 -1.029 2.245 1.00 31.39 ATOM 296 CB VAL 1511 -0.625 1.305 23.466 1.00 30.10 ATOM 297 CG1 VAL 1511 -0.625 1.305 23.466 1.00 30.10 ATOM 299 CV VAL 1511 -0.625 1.305 23.245 1.00 29.64 ATOM 300 O VAL 1511 -0.924 2.249 2.233 21.301 2.245 1.00 28.08 ATOM 301 N ALA 1512 -0.679 2.935 2.185 1.00 30.57 ATOM 302 CA ALA 1512 -0.679 2.935 21.057 1.00 25.23 ATOM 303 CB ALA 1512 -0.679 2.935 21.057 1.00 25.23 ATOM 304 C ALA 1513 -0.331 4.515 2.0061 1.00 27.06				-50,		07 -7	.728 28		1.00 50.39
ATOM 266 CZ ARG 1507 -8.012 -9.861 31.691 1.00 74.19 ATOM 268 NH2 ARG 1507 -7.193 -9.093 32.406 1.00 81.67 ATOM 269 C ARG 1507 -8.338 -1.1.068 32.134 1.00 82.38 ATOM 271 N VAL 1508 -7.190 -9.458 -3.340 28.611 1.00 36.16 ATOM 272 CA VAL 1508 -7.190 -2.335 28.782 1.00 36.16 ATOM 273 CE VAL 1508 -7.190 -2.335 28.782 1.00 36.16 ATOM 274 CG1 VAL 1508 -7.190 -2.335 28.782 1.00 36.19 ATOM 275 CG2 VAL 1508 -6.824 -1.296 29.883 1.00 30.19 ATOM 276 C VAL 1508 -5.948 -1.900 30.938 1.00 30.19 ATOM 277 O VAL 1508 -5.948 -1.900 30.938 1.00 34.68 ATOM 277 O VAL 1508 -5.392 -3.966 28.555 1.00 34.02 ATOM 278 N THR 1509 -5.427 -2.152 27.154 1.00 31.32 ATOM 280 CB THR 1509 -4.206 -2.527 26.476 1.00 30.47 ATOM 281 OG1 THR 1509 -5.427 -2.152 27.154 1.00 31.32 ATOM 282 CC THR 1509 -3.255 3.648 24.411 1.00 24.49 ATOM 283 C THR 1509 -3.255 3.648 24.411 1.00 24.49 ATOM 286 CA LYS 1510 -2.092 -1.432 26.893 1.00 29.17 ATOM 287 CB LYS 1510 -0.117 -0.460 29.135 1.00 27.29 ATOM 288 CG LYS 1510 -0.117 -0.460 29.135 1.00 27.29 ATOM 290 C LYS 1510 -0.117 -0.460 29.135 1.00 27.29 ATOM 291 NZ LYS 1510 -0.117 -0.460 29.135 1.00 27.29 ATOM 292 C LYS 1510 -0.117 -0.460 29.135 1.00 27.29 ATOM 293 O LYS 1510 -0.117 -0.460 29.135 1.00 28.74 ATOM 296 CB VAL 1511 -0.625 1.305 23.245 1.00 31.39 ATOM 297 CG1 VAL 1511 -0.625 1.305 23.245 1.00 31.39 ATOM 298 CG2 VAL 1511 -0.625 1.305 23.245 1.00 31.39 ATOM 299 C LYS 1510 -0.117 -0.460 29.135 1.00 29.64 ATOM 290 C LYS 1510 -0.117 -0.460 29.135 1.00 29.64 ATOM 290 C LYS 1510 -0.117 -0.460 29.135 1.00 29.64 ATOM 290 C LYS 1510 -0.521 -1.218 24.700 1.00 28.00 ATOM 291 NZ LYS 1510 -0.117 -0.460 29.135 1.00 30.19 ATOM 292 C LYS 1510 -0.521 -1.218 24.700 1.00 28.00 ATOM 293 O LYS 1510 -0.521 -0.235 2.615 1.00 31.39 ATOM 290 C LYS 1510 -0.521 -0.235 2.245 1.00 31.39 ATOM 290 C LYS 1510 -0.117 -0.460 29.135 1.00 29.64 ATOM 290 C LYS 1510 -0.521 -0.235 2.245 1.00 31.39 ATOM 290 C LYS 1510 -0.521 -0.235 2.245 1.00 31.39 ATOM 290 C LYS 1510 -0.521 -0.525 20.355 1.00 29.64 ATOM 290 C LYS 1510 -0.521 -0.525 20.23 20.23 2				-50,			.063 30		1.00 60.88
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ATOM 270		269			-8.3	38 - J.1.			00 81.67
ATOM 271 N VAL 1508		270			-8.98	32 - 3.			00 82.38
ATOM 273 CB VAL 1508		271				58 -3.3	354 27.		00 38.15
ATOM 273 CB VAL 1508		272							.00 36.46
ATOM 275 CG2 VAL 1508		273			-7.19		35 28. <sup>,</sup>		.00 35.19
ATOM 276 CG VAL 1508		274					<sup>196</sup> 29.8		.00 33.82
ATOM 276 C VAL 1508							23 30.4		.00 30.19
ATOM 278 N THR 1509			C VAL				00 30.9		.00 34.68
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ATOM 280 CB THR 1509		·-	_				<sup>26</sup> 28.5		00 33.91
ATOM 281 OG1 THR 1509	ATOM	279 <u>(</u>	CA THR		5.427		52 27.1		00 34.02
ATOM 282 CG2 THR 1509		-	B THR		-4.206		27 26.4		00 31.32
ATOM 283 C THR 1509		-					5 25.0		00 30.47
ATOM 284 C THR 1509		_	G2 THR				8 25.06		0.0 33 00
ATOM 285 N LYS 1510			THR				8 24.41	11 1.0	00 24 40
ATOM 285 N LYS 1510			THR		-3.323	-1.30	0 26.41	9 1.0	0 28 74
ATOM 287 CB LYS 1510			LYS			-0.21	9 26.03	9 1.0	00 27 20
ATOM 288 CG LYS 1510								3 1.0	0 29 17
ATOM 289 CD LYS 1510								1 1.0	0 30 55
ATOM 290 CE LYS 1510 1.191 -0.614 29.896 1.00 34.33  ATOM 291 NZ LYS 1510 1.065 -1.603 31.062 1.00 48.28  ATOM 292 C LYS 1510 0.318 -1.067 32.245 1.00 51.03  ATOM 293 O LYS 1510 -0.813 -0.213 25.355 1.00 29.64  ATOM 294 N VAL 1511 -0.904 1.004 24.836 1.00 30.10  ATOM 295 CA VAL 1511 -0.625 1.305 23.446 1.00 30.10  ATOM 296 CB VAL 1511 -1.951 1.464 22.636 1.00 31.39  ATOM 297 CG1 VAL 1511 -2.719 0.143 22.615 1.00 30.42  ATOM 299 C VAL 1511 -2.829 2.629 23.223 1.00 28.08  ATOM 299 C VAL 1511 0.274 3.346 24.360 1.00 30.51  ATOM 300 O VAL 1511 0.274 3.346 24.360 1.00 30.51  ATOM 301 N ALA 1512 0.679 2.935 22.185 1.00 28.30  ATOM 303 CB ALA 1512 1.408 4.173 21.979 1.00 25.23  ATOM 304 C ALA 1512 0.535 5.012 21.057 1.00 25.50  ATOM 305 O ALA 1512 0.031 4.515 20.061 1.00 27.06			LYS :					8 1.0	0 27 23
ATOM 291 NZ LYS 1510			) LYS 1					5 1.0	0 34 33
ATOM 292 C LYS 1510				510				5 1.00	0 40.49
ATOM 293 O LYS 1510			LYS 1	510	0 310			2 1.00	0 48.28
ATOM 294 N VAL 1511 -0.904 1.004 24.836 1.00 30.10 ATOM 295 CA VAL 1511 -0.625 1.305 23.446 1.00 30.10 ATOM 296 CB VAL 1511 -1.951 1.464 22.636 1.00 30.13 ATOM 297 CG1 VAL 1511 -2.719 0.143 22.615 1.00 30.42 ATOM 298 CG2 VAL 1511 -2.829 2.629 23.223 1.00 28.08 ATOM 300 O VAL 1511 0.150 2.626 23.365 1.00 30.51 ATOM 301 N ALA 1512 0.679 2.935 22.185 1.00 28.30 ATOM 303 CB ALA 1512 0.679 2.935 22.185 1.00 28.30 ATOM 304 C ALA 1512 0.535 5.012 21.979 1.00 25.23 ATOM 305 O ALA 1512 0.535 5.012 21.057 1.00 25.50 ATOM 306 N VAL 1513 0.351 6.352 20.061 1.00 27.06			Lys 1	510	-0.813		- · <b></b> -	1.00	51.03
ATOM 295 CA VAL 1511 -0.904 1.004 24.836 1.00 30.10  ATOM 296 CB VAL 1511 -0.625 1.305 23.446 1.00 30.13  ATOM 297 CG1 VAL 1511 -1.951 1.464 22.636 1.00 31.39  ATOM 298 CG2 VAL 1511 -2.719 0.143 22.615 1.00 30.42  ATOM 299 C VAL 1511 -2.829 2.629 23.223 1.00 28.08  ATOM 300 O VAL 1511 0.274 3.346 24.360 1.00 31.09  ATOM 301 N ALA 1512 0.679 2.935 22.185 1.00 28.30  ATOM 303 CB ALA 1512 1.408 4.173 21.979 1.00 25.23  ATOM 304 C ALA 1512 0.535 5.012 21.057 1.00 25.50  ATOM 305 O ALA 1512 0.033 4.515 20.061 1.00 27.06		204	_	510				1.00	29.64
ATOM 296 CB VAL 1511 -0.625 1.305 23.446 1.00 30.10  ATOM 297 CG1 VAL 1511 -1.951 1.464 22.636 1.00 31.39  ATOM 298 CG2 VAL 1511 -2.719 0.143 22.615 1.00 30.42  ATOM 299 C VAL 1511 -2.829 2.629 23.223 1.00 28.08  ATOM 300 O VAL 1511 0.274 3.346 24.360 1.00 30.51  ATOM 301 N ALA 1512 0.679 2.935 22.185 1.00 28.30  ATOM 303 CB ALA 1512 1.408 4.173 21.979 1.00 25.23  ATOM 304 C ALA 1512 0.535 5.012 21.331 1.00 23.82  ATOM 305 O ALA 1512 0.033 4.515 20.061 1.00 27.06				511				1.00	28.00
ATOM 297 CG1 VAL 1511 -1 951 1.464 22.636 1.00 30.13  ATOM 298 CG2 VAL 1511 -2.719 0.143 22.615 1.00 30.42  ATOM 299 C VAL 1511 -2.829 2.629 23.223 1.00 28.08  ATOM 300 O VAL 1511 0.274 3.346 24.360 1.00 30.51  ATOM 301 N ALA 1512 0.679 2.935 22.185 1.00 28.30  ATOM 303 CB ALA 1512 1.408 4.173 21.979 1.00 25.23  ATOM 304 C ALA 1512 2.740 3.889 21.331 1.00 23.82  ATOM 305 O ALA 1512 0.535 5.012 21.057 1.00 25.50  ATOM 306 N VAL 1513 0.351 6.352 20.061 1.00 27.06				511	-0.625		24.836	1.00	30.10
ATOM 298 CG2 VAL 1511 -2.719 0.143 22.615 1.00 31.39  ATOM 299 C VAL 1511 -2.829 2.629 23.223 1.00 28.08  ATOM 300 O VAL 1511 0.150 2.626 23.365 1.00 30.51  ATOM 301 N ALA 1512 0.679 2.935 22.185 1.00 28.30  ATOM 303 CB ALA 1512 1.408 4.173 21.979 1.00 25.23  ATOM 304 C ALA 1512 0.535 5.012 21.057 1.00 25.50  ATOM 305 O ALA 1512 0.033 4.515 20.061 1.00 27.06	3 000		VAL 1	511	-1 951	1.305	23.446	1.00	30.13
ATOM 299 C VAL 1511 -2.829 2.629 23.223 1.00 28.08 ATOM 300 O VAL 1511 0.274 3.346 24.360 1.00 30.51 ATOM 301 N ALA 1512 0.679 2.935 22.185 1.00 28.30 ATOM 303 CB ALA 1512 1.408 4.173 21.979 1.00 28.30 ATOM 304 C ALA 1512 2.740 3.889 21.331 1.00 25.23 ATOM 305 O ALA 1512 0.535 5.012 21.057 1.00 25.50 ATOM 306 N VAL 1513 0.351 6.332 20.061 1.00 27.06	30000		VAL 19	311	-2 719		22.636	1.00	31.39
ATOM 300 O VAL 1511	•			11	-2 829		22.615	1.00	30.42
ATOM 301 N ALA 1512 0.274 3.346 24.360 1.00 30.51 ATOM 302 CA ALA 1512 0.679 2.935 22.185 1.00 28.30 ATOM 303 CB ALA 1512 1.408 4.173 21.979 1.00 25.23 ATOM 304 C ALA 1512 2.740 3.889 21.331 1.00 23.82 ATOM 305 O ALA 1512 0.535 5.012 21.057 1.00 25.50 ATOM 306 N VAL 1513 0.351 6.302 20.061 1.00 27.06	3.55						23.223	1.00	28.08
ATOM 302 CA ALA 1512 0.679 2.935 22.185 1.00 31.09 ATOM 303 CB ALA 1512 1.408 4.173 21.979 1.00 25.23 ATOM 304 C ALA 1512 2.740 3.889 21.331 1.00 23.82 ATOM 305 O ALA 1512 0.535 5.012 21.057 1.00 25.50 ATOM 306 N VAL 1513 0.351 6.332 20.061 1.00 27.06		<u>.</u> .	VAL 15		0 274		23.365	1.00	30.51
ATOM 303 CB ALA 1512 1.408 4.173 21.979 1.00 28.30 ATOM 304 C ALA 1512 2.740 3.889 21.331 1.00 23.82 ATOM 305 O ALA 1512 0.535 5.012 21.057 1.00 25.50 ATOM 306 N VAL 1513 0.351 6.233 20.061 1.00 27.06	· · · · · · · · · · · · · · · · · · ·		ALA 15			3.346	24.360	1.00	31.09
ATOM 303 CB ALA 1512 2.740 3.889 21.331 1.00 25.23 ATOM 305 O ALA 1512 0.535 5.012 21.057 1.00 25.50 ATOM 306 N VAL 1513 0.351 5.02 20.061 1.00 27.06			ALA 15				22.185	1.00	28.30
ATOM 306 N VAL 1513 0.351 6.301 21.331 1.00 23.82 0.033 4.515 20.061 1.00 27.06	3/2011		ALA 15		2 740	4.173	21.979	1.00	25.23
ATOM 306 N VAL 1512 0.033 4.515 20.061 1.00 25.50 0.351 6.303	* mo						21.331	1.00	23.82
306 N VAL 1513 0.351 6.303 20.061 1.00 27.06	700		ALA 15		_		21.057	1.00	25.50
6.281 21.404 1.00 29.37	3 TOM	06 N				4.515	20.061	1.00	27.06
					331	0.281	21.404	1.00	29.37

MOTA	307	CA	VAL	1513	-0.477	7.199	20.625	1.00	31.53
ATOM	308	CB	VAL	1513	-1.588	7.843	21.504	1.00	32.26
ATOM	309	CG1	VAL	1513	-2.453	8.775	20.684	1.00	34.37
ATOM	310		VAL	1513	-2.452	6.776	22.152		33.42
MOTA	311	С	VAL	1513	0.347	8.328	20.006	1.00	33.34
MOTA	312	0	VAL	1513	1.030	9.064	20.719	1.00	32.35
ATOM	313	N	LYS	1514	0.321	8.423	18.680	1.00	36.65
MOTA	314	CA	LYS	1514	1.022	9.466	17.929	1.00	37.26
MOTA	315	CB	LYS	1514	1.541	8.917	16.606	1.00	36.21
MOTA	316	CG	LYS	1514	2.524	7.792	16.800	1.00	39.32
MOTA	317	CD	LYS	1514	2.725	6.998	15.535	1.00	42.59
ATOM	318	CE	LYS	1514	3.245	7.860	14.416	1.00	44.71
MOTA	319	NZ	LYS	1514	4.408	8.680	14.844	1.00	38.78
ATOM	320	С	LYS	1514	0.020	10.574	17.653	1.00	37.21
MOTA	321	0	LYS	1514	-1.095	10.305	17.192	1.00	37.39
ATOM	322	N	MET	1515	0.433	11.812	17.908	1.00	39.05
ATOM	323	CA	MET	1515	-0.419	12.981	17.713	1.00	41.68
ATOM	324	CB	MET	1515	-1.162	13.299	18.991	1.00	41.07
ATOM	325	CG	MET	1515	-0.251	13.641	20.139	1.00	40.69
ATOM	326	SD	MET	1515	-1.271	13.763	21.571	1.00	41.18
ATOM	327	CE	MET	1515	-1.523	12.018	21.959	1.00	40.98
ATOM	328	С	MET	1515	0.397	14.197	17.321	1.00	44.66
ATOM	329	0	MET	1515	1.606	14.255	17.550	1.00	43.83
ATOM	330	N	LEU	1516	-0.288	15.182	16.747	1.00	50.63
ATOM	331	CA	LEU	1516	0.349	16.423	16.312	1.00	52.21
ATOM	332	CB	LEU	1516	-0.513	17.129	15.255	1.00	50.18
MOTA	333	CG	LEU	1516	-0.757	16.463	13.904	1.00	50.25
ATOM	334	CD1	LEU	1516	-1.733	17.298	13.114	1.00	51.02
ATOM	335	CD2	LEU	1516	0.555	16.329	13.163	1.00	51.60
ATOM	336	C	LEU	1516	0.549	17.391	17.473	100	54.25
ATOM	337	0	LEU	1516	-0.143	17.326	19.488	1.00	52.52
MOTA	338	N	LYS	1517	1.500	18.299	17.302	1.00	59.09
MOTA	339	CA	LYS	1517	1.773	19.315	18.313		62.57
MOTA	340	CB	LYS	1517	3.220	19.813	18.222		66.29
ATOM	341	CG	LYS	1517	4.281	18.810	18.663	1.00	70.96
MOTA	342	CD	LYS	1517	5.666	19.197	18.130	1.00	74.61
ATOM	343	CE	LYS	1517	6.711	18.118	18.414		78.21
ATOM	344	NZ	LYS	1517	8.020	18.410	17.751	1.00	77.95
ATOM	345	С	LYS	1517	0.824	20.474	18.037		63.07
MOTA	346	0	LYS	1517	0.226	20.557	16.960		63.68
MOTA	347	N	SER	1518	0.720	21.391	18.987		64.54
ATOM	348	CA	SER	1518	-0.167	22.543	18.848		67.29
MOTA	349	CB	SER	1518	-0.085	23.439	20.090		65.14
MOTA	350	С	SER	1518	0.124	23.382	17.609		69.48
ATOM	351	0	SER	1518	-0.798	23.843	16.938		71.85
MOTA	352	N	ASP	1519	1.402	23.530	17.280		70.88
ATOM	353	CA	ASP	1519	1.802	24.326	16.127		72.00
MOTA	354	CB	ASP	1519	3.162	24.973	16.385		72.61
ATOM	355	C	ASP	1519	1.861	23.548	14.817		72.32
ATOM	356	0	ASP	1519	2.432	24.035	13.844		73.72
ATOM	357	N	ALA	1520	1.322	22.332	14.798		72.11
ATOM	358	CA	ALA	1520	1.344	21.508	13.595	1.00	71.13

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					386		
ATOM	359	СВ	Δ1.Δ	1520			

ATO	M	
	CB ALA 1520	0.659 20 173 13 0-5
ATO	יי 360 C או זא זייס 360 C	13.855 1 00 71 01
ATO	" 361 O ALA 1520	12.440 1 00 50 05
ATON	M 362 N TUD 1500	-0.314 22.962 12.639 1 00 71 47
ATOM	4 363 CA THE 1521	1.230 22.101 11 249 1 20 =
ATOM	364 CB TUD	0.6/6 22.726 10.064 7.00
ATOM	365 OG1 TUD 155	1.798 23.167 9.132 1.00 66.23
ATOM	366 000	2.521 22 016
ATOM	367 0	2.741 24 070
ATOM	368 0 707	-0.150 21 666
ATOM	369 N 222	-0.093 20 403 - 1.00 65.62
ATOM	370 Ch cres	-0.893 22 052
ATOM	271 05 1522	-1.698 21 005 3 1.00 63.60
ATOM	272 - 010 1522	-2.560 21 002
ATOM	222	-0.768 20.051 1.00 64.02
ATOM	274 - GEO 1522	-1.161 18 006 5.942 1.00 60.41
ATOM	374 N LYS 1523	0.475 20.443 6.738 1.00 61.94
ATOM	375 CA LYS 1523	1 440 6.662 1.00 56.47
ATOM	376 CB LYS 1523	2 730 23 6.080 1.00 54 53
ATOM	377 CG LYS 1523	3 907 10 5.713 1.00 57.44
ATOM	378 CD LYS 1523	3 482 70 5 219 1.00 61.49
ATOM	379 CE LYS 1523	4 601 17 25 4.071 1.00 64.66
ATOM	380 NZ LYS 1523	4 353 3.469 1.00 68.18
ATOM	381 C LYS 1523	1 720 10 2.458 1.00 73.23
ATOM	382 O LYS 1523	7.757 1.00 52.30
	383 N ASP 1524	6.832 1.00 54 50
ATOM ATOM	384 CA ASP 1524	8.376 1 00 47 70
ATOM	385 CB ASP 1524	2 300 45 55
	386 CG ASP 1524	2 744 25 10.783 1.00 47 64
ATOM ATOM	387 OD1 ASP 1524	2 040 20.311 10.817 1.00 49 50
ATOM	388 OD2 ASP 1524	4 715 11.460 1.00 47.22
ATOM	389 C ASP 1524	0.000 10.230 1.00 52.84
ATOM	390 O ASP 1524	9.661 1.00 43 55
ATOM	<sup>391</sup> N LEU 1525	10.007 1 00 42 00
ATOM	<sup>392</sup> CA LEU 1525	7.341 9.391 1.00 40.77
ATOM	393 CB LEU 1525	-2 701 9.483 1.00 40.28
ATOM	394 CG LEU 1525	74 100 9.411 1.00 40.54
ATOM	395 CD1 LEU 1525	-4 200 9.403 1.00 40 33
ATOM	396 CD2 LEU 1525	-5 120 -5 10.514 1.00 42.75
	397 C LEU 1525	9.524 1 00 36 00
ATOM	398 O LEU 1525	B.343 1 00 40 30
<b>5</b> — - ·	<sup>399</sup> N SER 1526	73 064 17.525 8.557 1.00 41.90
7	400 CA SER 1526	7.147 1 00 42 72
30000	401 CB SER 1526	-0.502 13.315 5.954 1.00 44.75
7 moss	402 OG SER 1526	-1 530 - 4.723 1.00 49.61
3 mass	<sup>403</sup> C SER 1526	4.352 1 00 50 07
T COOL	404 O SER 1526	0 207 42 6.144 1.00 42.71
	405 N ASP 1527	10.297 13.047 5.840 1.00 45 33
30000	106 CA ASP 1527	1.167 14.527 6.655 7 00 40 07
	107 CB ASP 1527	6.867 1.00 41 02
	08 CG ASP 1527	3.497 14.235 7.316 1.00 45 30
ATOM 4	09 OD1 ASP 1527	4.083 15.147 6.235 1.00 47 94
ATOM 4	10 OD2 ASP 1527	3.700 15.041 5.047 1.00 48.04
		4.957 15.966 6.600 1.00 49.11
0005.45		



ATOM	411	С	ASP	1527	1.782	12.485	7.858	1.00	39.01
MOTA	412	0	ASP	1527	2.021	11.298	7.651	1.00	40.04
MOTA	413	N	LEU	1528	1.094	12.917	8.909	1.00	35.93
ATOM	414	CA	LEU	1528	0.594	12.004	9.927	1.00	36.48
ATOM	415	CB	LEU	1528	-0.008	12.784	11.107	1.00	36.51
MOTA	416	CG	LEU	1528	-0.436	11.961	12.326	1.00	40.56
MOTA	417	CD1	LEU	1528	0.650	10.955	12.692	1.00	42.00
ATOM	418	CD2	LEU	1528	-0.770	12.877	13.499	1.00	38.25
ATOM	419	C	LEU	1528	-0.453	11.065	9.309	1.00	35.25
ATOM	420	0	LEU	1528	-0.442	9.855	9.566	1.00	36.37
MOTA	421	N	ILE	1529	-1.311	11.614	8.453		33.10
MOTA	422	CA	ILE	1529	-2.365	10.839	7.805		32.32
ATOM	423	CB	ILE	1529	-3.364	11.732	7.912		31.17
ATOM	424	CG2	ILE	1529	-4.311	10.861	6.1.87		32.01
ATOM	425	CG1	ILE	1529	-4.193	12.579	7.983	1.00	31.35
ATOM	426	CD1	ILE	1529	-5.024	13.662	7.335		32.59
MOTA	427	C	ILE	1529	-1.732	9.825	6.877		33.44
ATOM	428	0	ILE	1529	-2.148	8:667	õ.860	1.00	35.41
ATOM	429	N	SER	1530	-0.733	10.269	6.108	1.00	
ATOM	430	CA	SER	1530	0.007	9.414	5.171	1.00	34.34
ATOM	431	CB	SER	1530	1.126	10.197	4.495		38.37
MOTA	432	ΟG	SER	1530	0.605	11.332	3.835	1.00	
MOTA	433	C	SER	1530	0.614	8.208	5.968	1.00	30.41
MOTA	434	0	SER	1530	0.494	7.083	5.376		30.50
ATOM	435	N	GLU	1531	1.256	8.449	7.010		
ATOM	436	CA	GLU	1531	1.865	7.369	7.766		28.90
A'I'OM	437	CB	GLU	1531	2.629	7.907	8.973		
ATOM	438	CG	GLU	1531	3.263	6.812	9.825		29.33
ATOM	439	CD	GLU	1531	4.094	7.344	10.979	1.00	31.14
ATOM	440	OE1	GLU	1531	4.913	6.561	11.495	1.00	33.14
ATOM	441	OE2	GLU	1531	3.940	8.522	11.378	1.00	31.11
ATOM	442	C	GLU	1531	0.824	6.351	8.215		30.88
ATOM	443	0	GLU	1531	1.118	5.146	8.259	1.00	32.35
ATOM	444	N	MET	1532	-0.377	6.832	8.553	1.00	29.86
ATOM	445	CA	MET	1532	-1.476	5.966	8.996	1.00	30.01
ATOM	446	CB	MET	1532	-2.608	6.800	9.596	1.00	29.58
ATOM	447	CG	MET	1532	-3.761	5.968	10.146	1.00	31.20
MOTA	448	SD	MET	1532	-5.095	6.973	10.779	1.00	29.37
ATOM	449	CE	MET	1532	-5.271	8.228	9.489	1.00	21.59
ATOM	450	С	MET	1532	-2.002	5.145	7.814	1.00	29.60
ATOM	451	0	MET	1532	-2.131	3.923	7.893	1.00	29.68
ATOM	452	N	GLU	1533	-2.257	5.824	6.702	1.00	30.38
ATOM	453	CA	GLU	1533	-2.755	5.176	5.495	1.00	30.12
MOTA	454	CB	GLU	1533	-2.987	6.221	4.423		25.79
ATOM	455	CG	GLU	1533	-4.117	7.154	4.784	1.00	
MOTA	456	CD	GLU	1533	-5.420	6.405	5.064	1.00	
MOTA	457	OE1	GLU	1533	-5.923	5.696	4.166	1.00	
ATOM	458	OE2	GLU	1533	-5.939	6.518	6.197	1.00	
MOTA	459	С	GLU	1533	-1.787	4.120	5.003	1.00	
MOTA	460	0	GLU	1533	-2.197	3.043	4.563	1.00	
ATOM	461	N	MET	1534	-0.500	4.435	5.136	1.00	
ATOM	462	CA	MET	1534	0.606	3.571	4.737	1.00	
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7.0	TO L	
	FOM 463 CB MET 1534	1 00-
	OM 464 CG MET 153	4.305 4.985 1.00 22 24
	465 SD MET 1534	3.487 4.675 1 00 40
	OM 466 CE MET 1534	3.528 3.627 2 982 3 0
AT	OM 467 C MET 150	5.215 4.257 3 155 1 22
AT	OM 468 O MET 100	0.565 2.304 5 581
ATO	OM 469 N MET 355	0.596 1.193 5.050 3.50
ATO	OM 470 CR 155	0.493 2.485 6.896 3.00 33.24
ATC	OM 471 CT	0.417
ATC	)M 472 ~- 1335	0.325 1.000 28.82
ATO	OM 473 CD 100	1.622 2.43.
ATO	M 474 CR 1535	1.674 2 633 1.00 28.16
ATO	M 475 C 1535	1.393 4 225
ATO	M 476 0	-0.777 0.460 1.729 1.00 27.69
ATO	M 477	.0.682 -0.734445 1.00 28.59
ATOM	M 470 T LYS 1536	-1.885 1.070 7.530 1.00 30.37
ATON	470 CA LYS 1536	-3.078 0.315 7.019 1.00 26.53
ATOM	1 175 CB LYS 1536	-4.237 1.353 5.608 1.00 27.60
ATOM	1 491 CG LYS 1536	5.283 1.00 25 80
ATOM	1 422 - LYS 1536	-5 935 2 7 1.479 1.00 23 80
ATOM	102 CE LYS 1536	7.061 1.00 21 64
ATOM	104 LYS 1536	7 460 3.074 8.225 1.00 21 83
ATOM	LYS 1536	2 913 2 7.796 1.00 26.27
ATOM	LYS 1536	-3 150 -3 5.397 1.00 27 49
ATOM	1537	-2 10c - 3 393 1.00 29 21
ATOM	487 CA MET 1537	-1 890 1.00 27 89
ATOM	488 CB MET 1537	3.172 1 00 00 40
ATOM	489 CG MET 1537	2.085 1 00 32
	490 SD MET 1537	1.566 1 00 37 37
ATOM	491 CE MET 1537	0.303 0.744 1 00 42
ATOM	492 C MET 1537	
ATOM	493 C MET 1537	3,447 1 00 20 11
ATOM	494 N ILE 1538	2.996 1 00 00
ATOM	495 CA ILE 1538	4.223 1 00 00 -
ATOM	496 CB ILE 1538	1.189 -2.609 4.533 1.00 25
ATOM	497 CG2 ILE 1538	2.381 -1.948 5.280 ) 00 25 25
ATOM	498 CG1 ILE 1538	5.745 1 00 22 22
ATOM	499 CD1 ILE 1538	4.345 1 00 22
ATOM	500 C ILE 1538	4.445 -0.465 4.874 1 00 22
ATOM	501 O ILE 1538	0.756 -3.911 5.224 1.00 26 25
ATOM	502 N GLY 1539	1.2/4 -4.980 4.909 1 00 30 4
ATOM	503 CA GLY 1539	-0.200 -3.849 6.137 1.00 an
ATOM	504 C GLY 1539	-0.625 -5.069 6.812 1.00 25 -
ATOM	505 O GLY 1539	0.207 -5.369 8.039 1.00 26.88
ATOM	506 N LYS 1540	1.220 -4.708 P 301
ATOM	507 CA LYS 1540	-0.195 -6.396 8 788 3 88
ATOM	E00 an 1540	0.461 -6,781 10.052 1.00 23.25
ATOM	509 CC ***	-0.573 -7.350 11 029 1 21.53
ATOM	E10 1340	-1.530 -6.346 11 562 1
ATOM	533 210 1340	-2.542 .6.000
ATOM	510	-3.568 -5 042 1.00 36.24
ATOM	512 0	-2.973 -4.047 1.00 41.05
ATOM	514 0	1.577 -7.706
	514 O LYS 1540	1 536 0 700
		9.176 1.00 21.51
DOOM 1-		



			2.514 -7.670 10.905 1.00 19.82
	11	IS 1541	2.514 -7.070 -1.00 21.35
MOTA	515		3.622 -8.013 1 00 21 39
MOTA	310		4.704 -8.411 0.063 1.00 17.07
MOTA	517 0-		5.747 -9.430 1.00.18.04
MOTA	310		5.810 -10.007
MOTA	519 CD2 F		6.891 - 9.420 = 1.00.19.63
MOTA	520 ND1 H		7.609 -10.522 10.535 1.00 18 32
MOTA	521 CE1 I		6.975 -11.293 9.668 1.00 23 61
MOTA	522 NE2		4.198 -8.456 12.449 1.00 25 66
MOTA	222	HIS 1541	4 231 -7.352 13.002 1.00 23.00
MOTA		HIS 1541	4 507 -9.577 13.045 1.00 24.32
MOTA	J = -	LYS 1542	F 1/1 -9.610 14.390 1.00
MOTA	526 CA	LYS 1542	= 578 -11.044 14.742 1.90 30.70
ATOM	527 CB	LYS 1542	6 130 -11 239 16 150 1 34
MOTA	528 CG	LYS 1542	6 380 -12.719 16.420 1.00
ATOM	529 CD	LYS 1542	6 995 -13.414 15.183 1.00
ATOM	530 CE	LYS 1542	021 15 421 I.UU
	531 NZ	LYS 1542	2 624 14 608 1.00 24.59
ATOM	532 C	LYS 1542	5.52 5.676 1.00 23.35
MOTA	533 0	LYS 1542	5.402
MOTA	534 N	ASN 1543	7.147 - 702 13 689 1.00 21.40
ATOM	535 CA	ASN 1543	0.333
MOTA	536 CB	ASN 1543	9.550
MOTA	537 CG	ASN 1543	9.721
MOTA		1 ASN 1543	9.301 25 230 1.00 21.56
MOTA		2 ASN 1543	10.020 13 155 1.00 20.30
MOTA		ASN 1543	8.312 12 776 1.00 20.03
MOTA		ASN 1543	9.353 -5.733 180 1.00 20.02
MOTA		ILE 1544	7.153 .5.624 100 21.14
MOTA		3EAA	7.037 -4.220 -1 292 1.00 22.97
MOTA	544 CB	1544	3.34 1.00 23.27
MOTA		- 7544	7.436 -4.810 2010 1.00 22.85
MOTA	546 66	31 ILE 1544	5.082 -4.447 22 760 1.00 18.94
MOTA	(17	D1 ILE 1544	4.485 -3.974 1 00 20.02
MOTA		1544	6.044 -3.590 1.466 1 00 21.00
MOTA		1544	5.342 -4.303 221 1 00 20.09
MOTA		1545	6.103 2.273 23 1.00 22.82
1OTA		1545	5.140 -1.808 1.00 23.07
OTA	,	7.7.45	5.586 -0.101 - 20.21 94
OTA		·	4.399 0.632 25.193 1.00 20.49
OTA		G2 ILE 1545 G1 ILE 1545	6.759 -0.178 17 579 1.00 15.00
OTA	• •		6.450 -0.730 -4.010 1.00 24.18
OTA	-	DI	3.853 -1.555 11.60 1 00 25.68
OTA	111 2	15/5	3.809 -0.954 20.25 69
ATC	,,,,,	1546	2.829 -2.230 221 1 00 24 23
ATC	)(·)	1546	1.528 -2.311 13.853 1.00 25.21
TA	Ji	1546	0.866 -3.697 14.060 1.00 22 10
ATC	Ji-1 — — —	1546	3 600 -4.834 13.461 1.00 -
ATC	ъм 561	CG ASN 1546	1.764 -4.997 12.274 1.00 18 20
AT	ом 562	OD1 ASN 1546	2.324 -5.606 14.343 1.00 -
TA		ND2 ASN 1546	0.567 -1.235 14.325 1.00 24 14
	OM 564	C ASN 1546	0.709 -0.682 15.426 1.00 24.14
	OM 565	O ASN 1546	-0.382 -0.920 13.456 1.00 23.49
	OM 566	N LEU 1547	-

Δ.	TOM 567		
	mo	CA LEU 15	47 -1 417
	77011	CD +	47 0.069 13 718 3
	TOM 569	CC +	1.9/6 0.597 12 270
	TOM 570	CD1 LEU 15	1.535 12 252
Al	TOM 571	CD2 LEU 15	-2.834 2.903 12.923
	·OM 572	C LEU 15	-3.714 1.660 10.930
	'OM 573		-2.510 -0.681 14.405
AT	OM 574 1		-2.849 -1.823 14 160
AT	OM 575 (	-20 154	-3.017 -0.083 1.00 28.96
AT	OM 576 c		-4.047 -0.714
AT(	`M ~	154	8 -3.686 -0.692 10.365 1.00 22.37
ATC		0 134	8 -2.346 -1.360 -2.346 1.00 17.76
ATC		D1 LEU 154	8 -2 150 1 18.224 1.00 17.12
ATO		204	3 -2 266 2 777 19.708 1.00 18.81
ATO	M 500	154)	3 -5 305 -1/.631 1.00 16 20
ATO	M 505	220 1548	1 16.099 1.00 23 30
ATO	M 552 IV	221 1345	16.1/5 1.00 24 18
ATO	·	A GLY 1549	-6 536 13.758 1.00 21 53
ATON	4 ===	GLY 1549	13.485 1 00 22 45
ATOM		GLY 1549	3.421 15.340 1 00 34 33
ATOM	14	ALA 1550	3.835 15.163 1 00 25
ATOM	CA CA	ALA 1550	7.439 4.219 15.409 1 00 24 15
			5.672 15.313 1 00 32 34
ATOM	-05	ALA 1550	7.063 6.079 13 000
ATOM		ALA 1.550	0.802 6.415 15 200
ATOM	- TA	CYS 1551	5.707 5.876 15 pg.
ATOM	592 CA	CYS 1551	-8.383 7.660 16 313 1.00 26.43
ATOM	593 CB	CYS 1551	-9.425 8.590 1.6 cm
ATOM	5.94 SG	CYS 1551	-9.160 9.045 IR 127
ATOM	595 C	CYS 1551	-9.246 7.802 19.442
ATOM	596 O		-9.294 9.787 15 710 1.00 30.32
MOTA	597 N	-001	-8.364 10.575 15 028
ATOM	598 CA		10.145 9.823 14 763
ATOM	599 CB		-10.076 10.873 13.605
MOTA	C00 -	Mir.	-10.061 10.219 12 220
MOTA	603	-332	-11.266 9.465 12.280 1.00 30.58
ATOM	600 -		-8.895 9 355 12.096 1.00 31.11
ATOM	602 -	THR 1552	-11.241 11 847 12.151 1.00 27.59
ATOM	604	THR 1552	-11.192 12.017 13.695 1.00 32.24
ATOM	605	GLN 1553	-12.339 11 400 1.00 28.56
ATOM		GLN 1553	-13.529 12 222 -1.00 35.46
ATOM	607 -	GLN 1553	-14.775 11 350 14.295 1.00 38.72
ATOM		SLN 1553	14.148 1.00 38 66
ATOM		ELN 1553	-14 cor == 12.876 1.00 41 41
ATOM	C10		-15 442 11.627 1.00 44 05
ATOM	C 3 3	LN 1553	-13 746 11.445 1.00 45 0g
ATOM	C 4 A	LN 1553	-13 650 10.765 1.00 43 32
ATOM	~ ~ ~	LN 1553	-73 220 20 15.483 1.00 41 20
ATOM	613 N A	SP 1554	13.230 12.837 16.590 1 00 20 20
	614 CA AS	SP 1554	14.225 14.344 15.219 1 00 44 00
ATOM	615 CB AS		14.4/4 15.356 16.237 1 00 45
ATOM	616 CG AS		15.778 15.028 16.976 1 00 40
ATOM	617 OD1 AS		17.007 15.262 16.122 1 00 75
ATOM	618 OD2 AS	P 1554	-17.966 15.878 16.631 1.00 56.68
		-034	-17.030 14.020 -1.00 64.76
			14.829 14.947 1.00 60.79



ATOM	619	C	ASP	1554	-13.343	15.563	17.244	1.00 47.24
MOTA	620	0	ASP	1554	-13.522	15.375	18.452	1.00 48.98
MOTA	621	N	GLY	1555	-12.182	15.966	16.747	1.00 44.00
ATOM	622	CA	GLY	1555	-11.062	16.185	17.638	1.00 41.07
MOTA	623	С	GLY	1555	-9.728	15.891	16.994	1.00 40.26
ATOM	624	0	GLY	1555	-9.663	15.567	15.810	1.00 39.72
ATOM	625	N	PRO	1556	-8.635	15.987	17.759	1.00 39.21
ATOM	626	CD	PRO	1556	-8.634	16.266	19.208	1.00 39.09
MOTA	627	CA	PRO	1556	-7.271	15.740	17.294	1.00 37.84
MOTA	628	CB	PRO	1556	-6.436	15.947	18.549	1.00 39.66
ATOM	629	CG	PRO	1556	-7.269	16.842	19.389	1.00 39.53
ATOM	630	C	PRO	1556	-7.094	1.4.314	16.806	1.00 37.75
ATOM	631	0	PRO	1556	-7.574	13.377	17.444	1.00 37.25
MOTA	632	N	LEU	1557	-6.379	14.153	15.699	1.00 36.09
ATOM	633	CA	LEU	1557	-6.112	12.844	15.124	1.00 34.69
ATOM	634	CB	LEU	1557	-5.458	13.010	13.741	1.00 32.25
MOTA	635	CG	LEU	1557	-4.962	11.774	12.972	1.00 31.23
ATOM	636	CD1	LEU	1557	-6.080	10.763	12.715	1.00 25.69
ATOM	637	CD2	LEU	1557	-4.339	12.219	11.669	1.00 28.21
ATOM	638	C	LEU	1557	-5.190	12.057	16.060	1.00 34.59
ATOM	639	O	LEU	1557	-4.173	12.578	16.524	1.00 32.09
ATOM	640	Ŋ	TYR	1558	-5,606	10.841	16.396	1.00 32.63
MOTA	641	CA	TYR	1558	-4.796	9.993	17.237	1.00 29.66
MOTA	642	CB	TYR	1558	-5.529	9.630	18.534	1.00 33.14
MOTA	643	CG	TYR	1.558	-5.588	10.754	19.539	1.00 32.87
ATOM.	644	CD1	TYR	1558	-6.583	10.793	20.517	1.00 34.58
ATOM	645	CE1	TYR	1558	-5.678	11.957	21.407	1.00 34.65
MOTA	646	CD2	TYR	1558	-4.678	11.805	19.483	1.00 35.69
MOTA	647	CE2	TYR	1558	-4.760	12.878	20.367	1.00 37.01
MOTA	648	CZ	TYR	1558	· 5. <b>766</b>	12.899	21.324	1.00 37.52
MOTA	649	OH	TYR	1558	-5.868	13.986	22.164	1.00 40.19
MOTA	650	C	TYR	1558	-4.529	8.747	16.436	1.00 28.08
MOTA	651	0	TYR	1558	-5. <b>467</b>	8.137	15.924	1.00 30.12
ATOM	652	N	VAL	1559	-3.254	8.444	16.225	1.00 25 89
MOTA	653	CA	VAL	1559	-2.855	7.246	15.504	1.00 23.70
ATOM	654	CB	VAL	1559	-1.729	7.528	14.485	1.00 23.78
ATOM	655	CG1	VAL	1559	-1.456	6.282	13.623	1.00 20.75
ATOM	656	CG2	VAL	1559	-2.101	8.738	13.604	1.00 22.54
ATOM	657	С	VAL	1559	-2.358	6.311	16.596	1.00 23.47
MOTA	658	0	VAL	1559	-1.328	6.572	17.220	1.00 26.84
MOTA	659	N	ILE	1560	-3.146	5.283	16.889	1.00 23.58
MOTA	660	CA	ILE	1560	-2.818	4.316	17.928	1.00 23.75
MOTA	661	CB	ILE	1560	-4.112	3.732	18.552	1.00 22.67
MOTA	662	CG2	ILE	1560	-3.777	2.898	19.788	1.00 20.24
MOTA	663	CG1	ILE	1560	-5.063	4.884	18.904	1.00 20.09
ATOM	664	CD1	ILE	1560	-6.428	4.463	19.318	1.00 19.04
ATOM	665	C	ILE	1560	-1.954	3.181	17.356	1.00 27.39
ATOM	666	0	ILE	1560	-2.411	2.392	16.505	1.00 28.51
MOTA	667	N	VAL	1561	-0.720	3.089	17.840	1.00 26.76
ATOM	668	CA	VAL	1561	0.238	2.088	17.368	1.00 25.91
ATOM	669	CB	VAL	1561	1.445	2.801	16.653	1.00 24.50
ATOM	670	CG1	VAL	1561	0.952	3.480	15.397	1.00 13.55

_				
	ТОМ	671 CG	2 VAL 156	
	TOM	672 C	VAL 156	2.054 3.870 17 551
	TOM	573 O		0.693 1.151 19 510
	TOM (	574 N	-50	0.397 1.417 19 696
A:	rom e	75 CA		1.349 0 033 - 1.00 25.26
A	2014	76 CB		1.793 -0 901 - 1.00 22.30
	'OM 6	77 CG	-502	2.369 -2 170 10 -1.00 21.49
AT		78 CD		1.312 -3 135 10.630 1.00 16.65
AT	O		GLU 1562 GLU 1562	1.895 -4 356 18.092 1.00 19.71
AT	~		~	1.281 -5 422 -7 460 1.00 21.58
ATO	~	31 C		2,956 "4 360 1.00 24.28
ATO		. –	GLU 1562	2 802 10.825 1.00 23 74
ATO			GLU 1562	3.581 0.570
ATO	OM 68	_	TYR 1563	2 707 2 19./38 1.00 24 82
ATO		F	TYR 1563	3 677 - 21.422 1.00 26 96
ATO		6 00	TYR 1563	2 902 - 22 42.442 1.00 28 99
ATO			TYR 1563	3 744 2 23 /44 1.00 30 34
ATO			TYR 1563	4 457
ATO			TYR 1563	5 105 " 24.915 1.00 36 50
ATON			TYR 1563	3 707 26.021 1.00 36 go
ATON			TYR 1563	4 522 26.082 1.00 34 35
ATOM			YR 1563	5 210 27.186 1.00 34 42
ATOM		1	YR 1563	5 273 27.150 1 00 27 00
MOTA		• •	YR 1563	1.662 28.228 1 00
ATOM	0.74	O T	YR 1563	1.043 22.668 1.00
ATOM	055		LA 1564	2.745 -2.269 22.751 1 00 33
ATOM		CA AI	LA 1564	0.008 -0.440 22.779 1 00 21
ATOM	697	CB AI		7.303 1.192 22.998 1 00 1
ATOM	698	C AI		0.236 -1.026 21.792 1.00 30
ATOM	699	OAL		7.940 -0.663 24.283 1 00 25 25
ATOM	706	N SE		0.309 24.274 1 00 20
ATOM	701	CA SE		7.603 -1.303 25.389 1.00 22
ATOM	702	CB SE		26.712 1 00 20 25
ATOM	703	OG SE		-1.729 27.792 1 00 00
ATOM	704	C SEI		7.704 -3.094 27.611 1 00 33
ATOM	705	O SER		26.986 1 00 31 35
ATOM	706	N LYS		3.378 -0 150 27.902 1 00 35 5
ATOM	707	CA LYS		10.340 -1.576 26.229 1 00 30 30
		CB LYS		12.756 -1.560 26.495 1 00 20 00
MOTA	709	CG LYS		22.322 -2.973 26.447 1 00 20 25
ATOM		CD LYS		27.563 1 00 25 25
ATOM	711	CE LYS	1566	12.208 -5.279 27.459 1 00 25
ATOM		VZ LYS	1566	28.747
ATOM		LYS	1566	12.315 -7.421 28.716 1 00 37.41
ATOM	714 (		1566	12.529 -0.595 25.623 1.00 32.63
ATOM	715 N			25.756 -0.672 25.544 1.00 20 -
ATOM	716 C	A GLY	1567	11.799 0.322 24.979 1.00 30.89
ATOM	717 C		1567	12.423 1.328 24 120 -
ATOM	718 O		1567	13.136 0.874 22 P75
ATOM	719 N			12.919 -0.235 22 305
ATOM	720 C	- 1011	1568	14.011 1.731 22 352
ATOM	721 CI		1568	14.735 1.421 21 130 28.39
ATOM	722 CC		1568	15.188 2.698 20 410
		014	1568	16.396 3 353 20.418 1.00 30.32
0000				3.352 21.058 1.00 33.42





					2 720 21.317 1.00 35.16
			- 01	1568	17.418 2.720 22.0
MOTA	723	OD1	ASN	1568	16.328 4.661 21.203 2.00 28 34
ATOM	724	_		1568	15.884 0.443 21.314 1.00 30 67
ATOM	725	С	ASN	1568	16.478 0.373 22.388 1.00 27 65
ATOM	726	0	ASN	1569	16.212 -0.270 20.244 1.00 20.30 10
MOTA	727	N	LEU	1569	17.269 -1.270 20.247 1.00 27 49
ATOM	728	CA	LEU	1569	17.311 -1.974 18.880 1.00 28.82
MOTA	729	CB	LEU LEU	1569	18.292 -3.130 18.657 1.00 24.68
MOTA	730	CG	LEU	1569	18.236 -4.140 19.823 1.00 22.26
MOTA	731		LEU	1569	17.994 -3.791 20 676 1 00 29.37
ATOM	732		LEU	1569	18.667 =0.730 =0.755 1 00 29.72
MOTA	733	C	LEU	1569	19.389 -1.525 22-1 1 00 30.89
MOTA	734	0	ARG	1570	19.058 0.423
MOTA	735		ARG		20.374 0.943 20.121 1 00 30.95
MOTA	736		_		20.591 2.333 201 1 00 38.85
MOTA	737				21.896 2.963 20.203 1 00 43.03
ATOM	738		_		21.968 4.472 2010 1.00 53.34
MOTA	739				20.749 3.132 22 205 1 00 57.49
ATOM	740			0	20.404 5.575 20.055 1.00 55.59
ATOM	741				21.184 5.310 22.006 1 00 59.53
MOTA	742	_	II ARG	-	19.272 6.252 22.000 1 00 33.82
MOTA	74	_	AR		20.475 0.547 22.00 33.93
MOTA	74				21.351 0.250 22.5
MOTA	74				19.528 1.639 7.217 1 00 32.59
MOTA	74				19.435 1.746 24.317
MOTA	74		-		18.177 2.524 22.175 1 00 45.91
MOTA	74	_	B GI G GI		18.174 3.950 24 3.96 1.00 52.95
MOTA	74		D GI		16.822 4.634 24.50
MOTA	75		E1 GI		15.793 3.935 22 3 00 55.17
MOTA		_		เบ 1571	16.792 5.903 22.00 1.00 31.40
ATOM				LU 1571	19.380 0.361 2210 1.00 31.09
MOTA				LU 1571	20.115 0.034 23 1 00 29.24
MOTA			-	YR 1.572	18.503 -0.477 22.00 1.00 27.43
MOTA	_		• •	YR 1572	18.334 -1.833 221.
ATOM	_	_		YR 1572	17.387 -2.330 23.13
MOTA		58		YR 1572	17.196 -4.045 25.216 1.00 28.16
MOTA	-	159		YR 1572	16.224 -4.440 25.456 1.00 28.32
MOTA	_	760		TYR 1572	75.903 F 024 23.665 1.00 20.00
MOTA	•	761	CD2	TYR 1572	7.500 6 361 23.899 1.00 22.28
AOTA		762		TYR 1572	721 24 801 1.00 26.53
IOTA		763		TYR 1572	25 055 1.00 30.25
ATO		764		TYR 1572	2 564 24 960 1.00 30.90
ATO	-	765		TYR 1572	2 223 25,901 1.00 30.68
ATO		766		TYR 1572	2 227 23.933 1.00 31.27
OTA		767	N	LEU 1573	20.407
OTA OTA		768	CA	LEU 1573	21.776 2075 22.399 1.00 30.85
		769	CB	LEU 1573	22.207
OTA OTA		770	CG	LEU 1573	21.043
ATC		771		LEU 1573	5 272 21.695 1.00 25.82
)TA		772		LEU 1573	21.333 -2 390 24.791 1.00 36.07
ATC		773	C	LEU 1573	3 22.002 - 05.467 1.00 36.40
)TA )TA		774	0	LEU 1573	3 23.544 -3.117 25.457 1100
AI	<b>.</b>				

ATC		N GLN 157	4
ATO		CA GLN 157	22.013 -1,065 24 202
ATO		B GLN 157	23./63 -0.391 25 750
ATO		G GLN 157	23.722 1.119 25 522
ATO	٠,, ر		24.240 1.529 24 147
ATO	M 780 O	15/4	24.046 3.009 23.857 1.00 40.76
ATON	<sup>y</sup> 781 nm	70 At	23.391 3.740 24 502 1.00 44.73
ATOM	<sup>າ</sup> 782 ຕ	~	24.606 3.452 22 732
ATOM	<sup>1</sup> 783 0	~~-	23.502 -0.711 27 222 1 20 46.93
ATOM	784 N		24.431 -0.988 27 200
ATOM	785 CA	20,5	22,229 -0.740 -1.00 38.55
ATOM	786 CB	13/5	21.846 -1 001 -1.00 37.28
ATOM			20.394 -0.660
ATOM	788 O	ALA 1575	22.102 -2 473 23.178 1.00 31.42
ATOM	700	ALA 1575	21.758 -2.843 29.424 1.00 38.30
ATOM	700	ARG 1576	22 (42 30.544 1.00 47 11
ATOM	70-	ARG 1576	22 042 28.528 1.00 37 59
ATOM		ARG 1576	22 027 - 28.869 1.00 37 22
ATOM		ARG 1576	20 500 - 28.111 1.00 36 82
ATOM	793 CD	ARG 1.576	19 640 - 48.561 1.00 34 61
ATOM	794 NE	ARG 1576	19 300 -6.146 27.640 1.00 31 82
ATOM	795 CZ	ARG 1576	17 500 2 28.201 1.00 31 54
ATOM		ARG 1576	18 000 - 28.426 1.00 33 71
ATOM	797 NH2	ARG 1576	76 227 5.000 28.149 1.00 33 60
ATOM	798 C	ARG 1576	24 405 28.857 1.00 38 97
ATOM	799 O	ARG 1576	24 700 = 25.683 1.00 38 53
ATOM	800 N	ARG 1577	25 326 3.231 28.700 1.00 38 39
ATOM		ARG 1577	26.661 4.017 28.538 1.00 39 28
ATOM	802 CB	ARG 1577	27 206 - 28.394 1.00 39 32
ATOM	803 CG	ARG 1577	27.040 27.998 1.00 35.44
ATOM		ARG 1577	27 606 21 20 26 584 1 00 33 45
ATOM	^ ~ -	ARG 1577	27 700 21.042 26.330 1.00 32 83
ATOM		ARG 1577	29 204 24.897 1.00 36 69
ATOM	807 NH1 A	ARG 1577	29 710 24.384 1.00 36 99
ATOM	808 NH2 A	IRG 1577	25.175 1 00 40 25
ATOM	809 C A	RG 1577	23.065 1 00 36 50
ATOM		RG 1577	29.754 1 00 41 0.
ATOM		RO 1578	30.796 1 00 43 05
ATOM		RO 1578	29.769 1 00 44 05
ATOM	813 CA P	RO 1578	48,667 1 00 44
ATOM	814 CB P	RO 1578	20.8// -5.766 31.066 1.00 44.55
	815 CG PF	RO 1578	29.933 -6.809 30.686 1.00 42 45
700	816 C PF		29.327 1 00 43 65
ATOM	817 O PR	1578	29.490 -4.493 31.672 1 00 45 22
MOTA	818 N PR	•	23.814 -3.538 30.947 1 00 44 50
ATOM	819 CD PR		23.604 -4.432 33.003 1 00 46 7
3	820 CA PR		29.208 -5.463 33.981 1.00 45 5
	821 CB PR	-0,5	30.169 -3.265 33.685 1.00 47
ATOM 8	822 CG PR		30.175 -3.708 35.141 1.00 47.56
ATOM 8	323 C PRO		28.997 -4.638 35.205 1.00 45.45
	324 O PRO		31.575 -2.904 33.200 1.00 50 -2
ATOM 8	25 N ALA		32.481 -3.739 33 106
ATOM 8	26 CA ALA		19.097 -5.342 32 479 1 25
		1592	20 535 6 076
0000			32.445 1.00 59.47



MOTA 827 CB ALA 1592 20.975 -4.338 33.715 1.00 61.58 ATOM 828 С ALA 1592 21.367 -6.350 32.252 1.00 58.15 829 MOTA 0 ALA 1592 22.543 -6.285 31.879 1.00 59.09 ATOM B30 1.00 55.79 N ALA 1593 20.754 ..7.510 32.479 MOTA 1593 831 CA ALA 21.457 -8.775 32.324 1.00 55.06 ATOM 832 CB ALA 1593 20.519 -9.939 32.604 1.00 57.05 **ATOM** 833 С ALA 1593 22.053 -8.897 30.924 1.00 53.57 **ATOM** 834 0 ALA 1593 21.402 29.926 -8.598 1.00 53.85 **ATOM** 835 N GLN 1594 23.303 -9.336 30.862 1.00 53.22 24.004 MOTA 836 CA GLN 1594 -9.490 29.599 1.00 50.13 **ATOM** 837 CB GLN 1594 25.400 -10.082 29.832 1.00 50.73 MOTA 838 CG GLN 1594 26.308 -9.253 30.743 1.00 54.69 **ATOM** 839 CD GLN 1594 27.550 -10.019 31.217 1.00 57.79 **ATOM** 840 OE1 GLN 1594 28.075 -10.900 30.524 1.00 58.82 ATOM 841 NE2 GLN 1594 28.026 -9.673 32,407 1.00 59.53 1594 ATOM 842 C GLN 23.210 -10.374 28.637 1.00 47.73 ATOM 843 0 GLN 1594 22.427 -11.241 29.054 1.00 47.09 ATOM 844 N LEU 1595 23.418 -10.133 27.350 1.00 45.64 ATOM 845 CA LEU 1595 22.758 -10.880 26.292 1.00 42.00 MOTA 846 CB LEU 1595 22.405 -9.947 25.122 1.00 37.98 MOTA 847 CG LEU 1595 21.345 -8.894 25.446 1.00 37.70 ATOM 848 CD1 LEU 1595 21.568 .7.611 24.660 1.00 33.34 ATOM 849 CD2 LEU i.595 19.971 -9.479 25.222 1.00 32.84 ATOM 850 С LEU 1595 23.729 -11.944 25.828 1.00 40.92 ATOM 851 O LEU 1595 24.944 -11.745 25.855 1.00 41.12 **ATOM** 852 ij SER 1596 23.201 -13.103 25.471 1.00 40.09 ATOM SER 853 CA 1596 24.044 -14.178 24.985 1.00 38.93 ATOM 854 CB SER 1596 23.388 -15.535 25.235 1.00 37.45 **ATOM** 855 OG SER 1596 22.158 -15.662 24.545 1.00 39.49 ATOM 856 C SER 1596 24.302 -13.987 23.499 1.00 39.41 MOTA 857 0 SER 1596 23.634 -13.183 22.832 1.00 39.51 ATOM 858 N SER 1597 1.00 39.17 25.266 -14.738 22.977 **ATOM** 859 CA SER 1597 25.587 -14.667 21.563 1.00 40.23 ATOM 860 CB SER 1597 26.740 -15.611 21.230 1.00 39.96 ATOM 861 ЭG SER 1597 27.865 -15.339 22.048 1.00 46.60 **ATOM** 862 3 SER 1597 24.347 -15.057 20.773 1.00 39.65 ATOM 1597 863 0 SER 24.066 -14.469 19.725 1.00 41.13 ATOM 864 N LYS 1598 23.590 -16.023 21.291 1.00 36.82 **ATOM** 865 CA LYS 1598 22.390 -16.467 20.611 1.00 36.17 ATOM 866 CB LYS 1598 21.827 -17.742 21.217 1.00 36.19 ATOM 867 CG LYS 1598 21.030 -18.562 20.180 1.00 39.59 MOTA 868 CD LYS 1598 20.150 -19.623 20.830 1.00 37.49 869 **ATOM** CE LYS 1598 19.769 -20.719 19.855 1.00 39.64 ATOM 870 NZ LYS 1598 20.976 -21.437 19.380 1.00 41.43 MOTA 871 C LYS 1598 21.340 -15.381 20.649 1.00 37.72 ATOM 872 O LYS 20.604 -15.213 1598 19.677 1.00 39.82 **ATOM** 873 N ASP 1599 21.291 -14.627 21.752 1.00 36.20 MOTA 874 CA ASP 1599 20.331 -13.530 21.907 1.00 33.96 MOTA 875 CB **ASP** 1599 20.456 -12.884 23.279 1.00 35.66 **ATOM** 876 CG **ASP** 1599 19.913 -13.744 24.394 1.00 36.18 **ATOM** 877 OD1 ASP 1599 20.365 -13.565 25.544 1.00 39.14 ATOM 878 OD2 ASP 1599 19.036 -14.593 24.128 1.00 33.40





	MO	879 C	ASP 1599	
AT		880 O		20.595 -12.471 20 857 1 66 -
AT	~	881 N		19.660 -11.953 20 225
ATC		882 CA	LEU 1600	21.871 -12 122
ATO		883 CB	LEU 1600	22.304 -11 123
ATO			LEU 1600	23.804 -10.950 1.00 31.14
ATO			LEU 1600	24.174 +10 153 00 1.00 30.23
ATO			LEU 1600	25.660 -0.077
ATO		86 CD2	LEU 1600	23.408 -9.057 21.324 1.00 24.11
ATO		187 C	LEU 1600	21 964 21.369 1.00 21.94
ATO			LEU 1600	21 205 12.523 18.291 1.00 29.24
			VAL 1601	22 272
ATO			VAL 1601	21 002 17.930 1.00 27 38
ATO			VAL 1601	22 642 16.597 1.00 27 26
ATO	_	92 CG1 '	VAL 1601	+ <del>-</del>
ATON		93 CG2 1	/AL 1601	22.403 -15.104 14 921
ATOM		· -	/AL 1601	24.156 -14.568 16 503 1
ATOM		\ <b>-</b>	/AL 1601	20.4/4 -13.353 16 300 3 00
MOTA	. 0)		ER 1602	19.991 -13.147 15 295 1 22
ATOM	98			19.733 -13.590 17.479 1 00
ATOM		<u> </u>		18.277 -13.671 17 406 1 22
ATOM	89			17.731 -14.259 18 604
ATOM	900	^ ~		16.317 -14.306 18 646 1 00 29.02
ATOM	903	1 -		17.669 -12.280 17 149 1 20
ATOM	902	`		16.643 -12.141 16.465 1.00 26.87
ATOM	903			18.289 -11 262
ATOM	904			17.878 -9.073
ATOM	905			18.797 9 937
ATOM	906			18 512 7 20.330 1.00 23.87
ATOM	907			17.994 0 515
ATOM	908	- 01		17.083 -0.000 1.00 25.24
ATOM	909			19.138 -9.054 -1.00 27.48
ATOM	910			19.422 -9.502 - 20.80
ATOM	911			20.851 -10.000
ATOM	912		- <del>-</del>	18 419 -10 700
ATOM	913			17.894 0 713
ATOM	914			18.130 -11 555
ATOM	915			17.175 -12.250
ATOM	916	CB TYR		17.104 -13 753
ATOM	917			15.997 -14 600 1.00 27.35
ATOM	918	CD1 TYR		16.109 -15 244
ATOM	919			15.069 -16.046
ATOM	920	CD2 TYR		14 830 -14 707
ATOM	921	CE2 TYR	1605	13.801 -15 505
ATOM	922	CZ TYR	1605	13.922 -16.220
ATOM	923	OH TYR	1605	12.855 -16.04
ATOM		C TYR	1605	15 766 11 77-
ATOM		O TYR	1605	15 190 33 63-
ATOM		N GLN	1606	15 227 74 8
ATOM		CA GLN	1606	13.907 -10.600 13.807 1.00 27.12
ATOM	<b>-</b> -	CB GLN	1606	13 561 -10 202 13.892 1.00 25.32
ATOM		CG GLN	1606	13 329 -11 600 15.342 1.00 24.31
ATOM		CD GLN	1606	13 052 -11 242 16.210 1.00 25.05
014	930	DE1 GLN	1606	12 087 10 549 1.00 26.35
				12.08/ -10.542 17.944 1.00 26.11
CCCD /==-				

ATOM	931	NE2	GLN	1606	13.917	-11.684	18.551	1.00 27.77
MOTA	932	С	GLN	1606	13.849	-9.415	13.078	1.00 27.52
MOTA	933	0	GLN	1606	12.825	-9.089	12.455	1.00 27.87
ATOM	934	N	VAL	1607	14.943	-8.662	13.122	1.00 27.90
ATOM	935	CA	VAL	1607	15.053	-7.419	12.359	1.00 26.41
ATOM	936	CB	VAL	1607	16.337	-6.661	12.731	1.00 25.61
ATOM	937	CG1	VAL	1607	16.545	-5.457	11.800	1.00 27.37
ATOM	938	CG2	VAL	1607	16.277	-6.224	14.190	1.00 21.50
ATOM	939	С	VAL	1607	15.035	-7.718	10.860	1.00 26.09
ATOM	940	0	VAL	1607	14.337	-7.046	10.096	1.00 28.48
ATOM	941	N	ALA	1608	15.795	-8.722	10.435	1.00 23.05
ATOM	942	CA	ALA	1608	15.812	-9.079	9.027	1.00 20.32
ATOM	943	CB	ALA	1608	16.823	-10.145	8.783	1.00 14.95
MOTA	944	C	ALA	1608	14.418	-9.558	8.600	1.00 23.08
ATOM	945	0	ALA	1608	14.033	-9.405	7.432	1.00 23.91
ATOM	946	N	ARG	1609	13.671	-10.169	9.530	1.00 24.57
ATOM	947	CA	ARG	1609	12.314	-10.628	9.246	1.00 24.30
MOTA	948	CB	ARG	1609	11.822	-11.577	10.326	1.00 26.13
MOTA	949	CG	ARG	1609	12.278	-12.979	10.114	1.00 31.07
ATOM	950	CD	ARG	1609	11.449	-13.885	10.939	1.00 36.13
ATOM	951	NE	ARG	1609	10.771	-14.865	10.115	1.00 38.37
MOTA	952	CZ	ARG	1609	9.931	-15.778	10.594	1.00 37.95
ATOM	953	NHl	ARG	1609	9.674	-15.828	11.898	1.00 35.31
ATOM	954	NH2	ARG	1609	9.353	-16.649	9.776	1.00 37.85
MOTA	955	C	ARG	1609	11.318	-9.490	9.065	1.00 22.34
ATOM	956	0	ARG	1609	10.470	-9.542	8.160	1.00 24.57
MOTA	957	N	GLY	1610	11.375	-8.500	9.948	1.00 20.52
MOTA	958	CA	GLY	1610	10.497	-7.353	9.827	1.00 19.33
ATOM	959	С	GLY	1610	10.732	-6.715	8.464	1.00 20.04
ATOM	960	0	GLY	1610	9.794	-6.455	7.693	1.00 19.10
ATOM	961	N	MET	1611	12.011	-6.545	8.130	1.00 18.21
MOTA	962	CA	MET	1611	12.423	-5.970	6.851	1.00 20.32
MOTA	963	CB	MET	1611	13.925	-5.737	6.838	1.00 19.20
MOTA	964	CG	MET	1611	14.371	-4.547	7.694	1.00 20.83
MOTA	965	SD	MET	1611	13.449	-2.960	7.422	1.00 25.39
MOTA	966	CE	MET	1611	13.869	-2.525	5.757	1.00 18.67
ATOM	967	C	MET	1611	12.024	-6.843	5.670	1.00 23.98
MOTA	968	0	MET	1611	11.608	-6.332	4.613	1.00 24.13
MOTA	969	N	GLU	1612	12.141	-8.162	5.825	1.00 25.76
MOTA	970	CA	GLU	1612	11.759	-9.059	4.743	1.00 25.49
ATOM	971	CB	GLU	1612		-10.522	5.110	1.00 26.09
ATOM	972	CG	GLU	1612		-11.468	3.968	1.00 26.56
ATOM	973	CD	GLU	1612		-12.942	4.313	1.00 29.26
ATOM	974		GLU	1612		-13.316	5.448	1.00 29.10
ATOM	975		GLU	1612		-13.725	3.443	1.00 31.11
ATOM	976	С	GLU	1612	10.283	-8.821	4.398	1.00 26.29
ATOM	977	0	GLU	1612	9.916	-8.728	3.226	1.00 28.46
MOTA	978	N	TYR	1613	9.437	-8.700	5.422	1.00 24.78
ATOM	979	CA	TYR	1613	8.003	-8.456	5.212	1.00 23.07
MOTA	980	CB	TYR	1613	7.263	-8.526	6.549	1.00 23.75
MOTA	981	CG	TYR	1613	5.785	-8.218	6.449	1.00 20.80
ATOM	982	CD1	TYR	1613	4.880	-9.213	6.062	1.00 20.97

ATO	<b>Σ</b> Μ		_		
ATC		983	CE1		3.517 -8.944 5.958 1.00 20 03
ATC		984		YR 1613	5.330 1.00 20.03
ATC		985		YR 1613	3 926 6 44
ATO	-	86		YR 1613	3 046 2 55
ATO		87		YR 1613	1.604 7.100 24.87
				YR 1613	7 766 7 000
ATO	• •			YR 1613	5 970 5 970
ATO				EU 1614	9.436
ATO			CA L	EU 1614	8 321 4 722
ATO				EU 1614	9 150 20.42
ATO				EU 1614	8 607 2 205 5 5 1.00 17.68
ATON		94 (	CD1 LE	EU 1614	9 504 -2 425
ATON			CD2 LE	U 1614	7.230 -2.705
ATOM		_	LE		P 720 14.07
ATOM		_	) LE		8 073
ATOM		_	AL		9 910 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5
ATOM		_	A AL	A 1615	10 313 5 13 1.00 21.55
ATOM	-	_	B AL	A 1615	11 625 6 255
ATOM		_	AL	A 1615	9 264 6 222 1.00 19.78
ATOM		_	AL.		0.451 1.00 19.98
ATOM	-		SE		P 603
ATOM			A SEI	R 1616	7.660 7.660 7.665
ATOM	100		B SEI		7 282 0 215
ATOM	1006		3 SEF	1616	6 415 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2
ATOM	100	_	SEF	1616	6 397 7 255
ATOM	1008	_	SEF	1616	5 650 7 00-
ATOM	1009		LYS	1617	6 126 6 127 1.00 23.62
ATOM	1010	) CA	LYS	1617	1.00 23.39
ATOM	1011		LYS	1617	1.00 23.02
ATOM	1012	CG	LYS	1617	3 700
ATOM	1013		LYS	1617	2 462 6 115 1.00 24.94
ATOM	1014	CE	LYS	1617	1 691 7 575
ATOM	1015	NZ	LYS	1617	2 401 2 252
ATOM	1016	C	LYS	1617	5 346 2 2 2 3 3 7 3
ATOM	1017	0	LYS	1617	4 500 2 22
ATOM	1018	N	LYS	1618	6 496
ATOM	1019	CA	LYS	1618	6 057 0 000
ATOM	1020	CB	LYS	1618	5 071 1.00 24.05
ATOM	1021	CG	LYS	1618	5 724 2 462
ATOM	1022	CD	LYS	1618	5.749 1.00 28.34
ATOM	1023	CE	LYS	1618	E 500
ATOM	1024	NZ	LYS	1618	4 373
ATOM	1025	С	LYS	1618	7 404 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5
ATOM	1026	0	LYS	1618	7 522 2 5.750 1.00 23.84
ATOM	1027	N	CYS	1619	7 770 7 770
ATOM	1028	CA	CYS	1619	P 103
ATOM	1029	CB	CYS	1619	7 330
ATOM	1030	SG	CYS	1619	7 036 1.00 20.84
ATOM	1031	C	CYS	1619	0.507 1.00 26,69
ATOM	1032	0	CYS	1619	10 252 1 125
ATOM	1033	N	ILE	1620	10 110 0 755
ATOM	1034	CA	ILE	1620	11 522 1.288 1.00 23.91
					11.532 1.046 1.474 1.00 26.01

ATOM	1035	CB	ILE	1620	12.098	1.830	0.236	1.00	22.61
MOTA	1036	CG2	ILE	1620	13.551	2.259	0.471	1.00	16.86
ATOM	1037	CG1	ILE	1620	12.014	0.977	-1.026	1.00	22.72
ATOM	1038	CD1	ILE	1620	12.096	1.804	-2.316	1.00	23.62
MOTA	1039	C	ILE	1620	11.566	1.934	2.729	1.00	26.83
ATOM	1040	0	ILE	1620	10.900	2.965	2.772	1.00	28.92
MOTA	1041	N	HIS	1621	12.293	1.500	3.758	1.00	26.44
MOTA	1042	CA	HIS	1621	12.386	2.245	5.007	1.00	23.61
ATOM	1043	CB	HIS	1621	13.142	1.429	6.065	1.00	20.98
ATOM	1044	CG	HIS	1621	12.940	1.917	7.463	1.00	21.57
ATOM	1045	CD2	HIS	1621	12.321	1.346	8.528	1.00	20.74
ATOM	1046	ND1	HIS	1621	13.382	3.151	7.897	1.00	21.08
MOTA	1047	CE1	HIS	1621	13.035	3.321	9.162	1.00	21.00
MOTA	1048	NE2	HIS	1621	12.396	2.237	9.572	1.00	21.97
MOTA	1049	C	HIS	1621	13.054	3.582	4.841	1.00	24.83
MOTA	1050	0	HIS	1621	12.560	4.585	5.310	1.00	25.76
ATOM	1051	N	ARG	1622	14.247	3.565	4.269	1.00	27.57
ATOM	1052	CA	ARG	1622	15.056	4.776	4.066	1.00	26.47
ATOM	1053	CB	ARG	1622	14.233	5.918	3.460		20.08
ATOM	1054	CG	ARG	1622	13.762	5.634	2.077	1.00	15.87
ATOM	1055	CD	ARG	1622	12.998	6.791	1.501	0.50	11.86
ATOM	1056	NE	ARG	1622	12.613	6.458	0.144		12.46
MOTA	1057	CZ	ARG	1622	11.537	5.748	-0.178		11.18
ATOM	1058	NHl	ARG	1622	10.711	5.304	0.767	0.50	7.16
ATOM .	1059	NH2	ARG	1622	11.340	5.398	-1.442	0.50	9.57
ATOM	1060	C	ARG	1622	15.813	5.250	5.325	1.00	26.18
MOTA	1061	0	ARG	1622	16.645	6.150	5.250		26.90
MOTA	1062	N	ASP	1623	15.544	4.650	6.480		27.26
ATOM	1063	CA	ASP	1623	16.268	5.042	7.684		29.80
ATOM	1064	CB	ASP	1623	15.714	6.330	8.292		32.13
ATOM	1065	CG	ASP	1623	16.690	6.940	9.298	1.00	37.87
MOTA	1066	OD1	ASP	1623	16.237	7.671	10.202	1.00	42.95
MOTA	1067	OD2	ASP	1623	17.907	6.684	9.191	1.00	41.09
ATOM	1068	С	ASP	1623	16.364	3.943	8.738	1.00	29.10
ATOM	1069	0	ASP	1623	16.164	4.168	9.939	1.00	27.69
MOTA	1070	N	LEU	1624	16.723	2.755	8.270	1.00	28.23
MOTA	1071	CA	LEU	1624	16.874	1.599	9.129	1.00	26.00
ATOM	1072	CB	LEU	1624	16.944	0.351	8.245		22.14
MOTA	1073	CG	LEU	1624	17.036	-0.998	8.941	1.00	22.32
ATOM	1074	CD1	LEU	1624	15.853	-1.196	9.932	1.00	17.01
ATOM	1075	CD2	LEU	1624	17.068	-2.064	7.848	1.00	20.50
ATOM	1076	С	LEU	1624	18.129	1.757	10.003		25.89
ATOM	1077	0	LEU	1624	19.247	1.917	9.499	1.00	
ATOM	1078	N	ALA	1625	17.930	1.706	11.316	1.00	
ATOM	1079	CA	ALA	1625	19.006	1.864	12.292	1.00	
MOTA	1080	CB	ALA	1625	19.323	3.340	12.493	1.00	
ATOM	1081	С	ALA	1625	18.475	1.286	13.584	1.00	
ATOM	1082	0	ALA	1625	17.269	1.083	13.721	1.00	
ATOM	1083	N	ALA	1626	19.357	1.041	14.543	1.00	
ATOM	1084	CA	ALA	1626	18.929	0.491	15.827	1.00	
ATOM	1085	CB	ALA	1626	20.148	0.145	16.691	1.00	
ATOM	1086	C	ALA	1626	18.015	1.474	16.560	1.00	
		-		<del></del>			_0.500	2.00	13

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ATC ATC		087		ALA	1626	17.	184	1.06	59 17 7			
ATC		880		ARG	1627	18.1		2.77			. 00	26.38
ATO		089		ARG	1627	17.3		3.78			.00	23.08
ATO		90		ARG	1627	17.8		5.18			.00	24.05
ATO		91		<b>A</b> RG	1627	17.7		5.50			.00	28.05
ATO.		92		<b>I</b> RG	1627	18.1		6.92				37.58
ATO				<b>I</b> RG	1627	18.4		7.08			.00	42.10
ATO				<b>LRG</b>	1627	19.6		7.00			.00	42.67
ATO			NH1 A		1627	20.7		6.75			.00	43.58
ATO			NH2 A		1627	19.8		7.20				46.17
ATO				RG	1627	15.9		3.632			.00	43.78
ATON	_			RG	1627	15.0		3.979			00	23.04
ATOM				SN	1628	15.72		3.093				22.27
ATOM	,	_		SN	1628	14.38		2.934			00	24.49
ATOM				SN	1628	14.35		3.407			00 :	23.80
ATOM		_		SN	1628	14.50		1.918		_		27.82
ATOM	_ •		D1 A9		1628	13.87		5.686			00 3	30.25
ATOM		-	D2 AS		1628	15.36		348			00 3	32.33
ATOM	_				1628	13.78		.524	14.83			1.50
ATOM	_	_			1628	12.89		.161				3.93
ATOM	110	_	• •		1629	14.30	_	.733	14.056			3.64
ATOM	110			L	1629	13.77	_	.610	15.763			4.10
ATOM	110				1629	14.829		.727	16.036		0 2	2.59
ATOM	111		G1 VA		1629	14.346		.014	15.823 16.462		0 2	1.16
ATOM	1111	_	32 VA		1629	15.068		.962	14.341		0 1	7.53
ATOM	1112		VA:		L629	13.411		.575	17.520			4.48
ATOM	1113	_	VA		629	14.237		.204	18.357	-		4.81
ATOM	1114		LE		.630	12.181		941	17.850			1.09
ATOM	1115			_	.630	11.751		919	19.239		0 24	
ATOM	1116				630	10.447		129	19.359		0 26	5.53
ATOM	1117				630	10.522		293	18.758	1.0	0 26	.19
ATOM	1118		1 LEU		630	9.149		870	18.601		0 24	
ATOM	1119		2 LEU		630	11.339		196	19.618	1.00	0 20	.51
ATOM	1120	C	LEU		630	11.641		327	19.835	1.00	) 19	.77
ATOM	1121	0	LEU	_	630	11.475		320	19.108	1.00	, 28	.14
ATOM	1122	N	VAL	1	631	11.792	-2.		21.153	1.00		
ATOM	1123 1124	CA	VAL		531	11.741	-3.		21.866	1.00		.21
ATOM		CB	VAL		531	13.068	-3.		22.624	1.00		. 96
ATOM	1125		VAL		531	13.113	-5.:		23.222	1.00	25	. 71
ATOM	1126 1127		VAL		31	14.240	-3.6		21.680	1.00	20.	.40
ATOM	1128	C	VAL		31	10.560	-3.7		22.836	1.00	19.	. 88
ATOM	1128	0	VAL		31	10.419	-2.9		23.738	1.00	29.	84
ATOM	1130	N	THR		32	9.703	-4.7		22.641	1.00	32.	46
ATOM	1131	CA	THR		32	8.530	-4.9		23.487	1.00	30.	90
ATOM		CB	THR	16		7.476	-5.8		22.793	1.00	31.	16
ATOM	1132		THR	16		7.948	-7.1		22.708	1.00	∠9.	58
ATOM	1133	CG2		16		7.186	-5.2		21.414	1.00	29.	17
ATOM	1134	C	THR	16	32	8.882	-5.6		24.809	1.00	22.	23
MOTA	1135	0	THR	16	32	9.950	-6.1		4.809 4.946	1.00	32.	23
ATOM	1136	N	GLU	16		7.946	-5.5	_	5.751	1.00	33.	23
ATOM	1137	CA	GLU	16:		8.165	-6.1			1.00	34.	38
1014	1138	CB	GLU	163	33	6.881	-6.1			1.00	35.	51
								- 2		1.00	35.4	18

ATOM	1139	CG	GLU	1633	7.004	-6.685	29.309	1.00	45.16
ATOM	1140	CD	GLU	1633	8.070	-5.999	30.183	1.00	50.45
MOTA	1141	OE1	GLU	1633	8.174	-4.750	30.163	1.00	52.70
MOTA	1142	OE2	GLU	1633	8.789	-6.723	30.919	1.00	53.59
MOTA	1143	С	GLU	1633	8.624	-7.635	26.930	1.00	35.40
ATOM	1144	0	GLU	1633	9.387	-8.119	27.758	1.00	36.57
ATOM	1145	N	ASP	1634	8.204	-8.308	25.861		36.76
ATOM	1146	CA	ASP	1634	8.573	-9.709	25.662		37.95
MOTA	1147	CB	ASP	1634		-10.491	24.991		42.90
MOTA	1148	CG	ASP	1634		-10.315	25.706		49.06
ATOM	1149	OD1	ASP	1634		-10.957	26.759		50.95
ATOM	1150		ASP	1634	5.256	-9.544	25.197		53.92
ATOM	1151	С	ASP	1634	9.842	-9.882	24.840	1.00	
ATOM	1152	0	ASP	1634		-10.988	24.414	1.00	
ATOM	1153	N	ASN	1635	10.582	-8.787	24.655		36.53
ATOM	1154	CA	ASN	1635	11.833	-8.763	23.868		
ATOM	1155	СВ	ASN	1635	12.893	-9.692	24.471	1.00	
ATOM	1156	CG	ASN	1635	13.335	-9.244	25.840		37.91
ATOM	1157		ASN	1635	13.496	-8.057			37.60
ATOM	1158		ASN	1635		-10.191	26.088		42.72
ATOM	1159	C	ASN	1635	11.641		26.743		38.03
ATOM	1160	0	ASN	1635		-9.073	22.372		34.59
ATOM	1161	N	VAL		12.431	-9.799	21.754		33.52
ATOM	1162		VAL	1636	10.557	-8.541	21.819		31.95
ATOM		CA		1636	10.260	-8.722	20.415		28.92
ATOM	1163	CB	VAL	1636	8.743	-8.945	20.177		31.00
	1164		VAL	1636	8.451	-9.066	18.678		29.52
ATOM ATOM	1165		VAL	1636		-10.220	20.884		29.03
ATOM	1166	C	VAL	1636	10.725	-7.461	19.721		28.05
ATOM	1167	0	VAL	1636	10.432	-6.355	20.179		25.21
	1168	N	MET	1637	. 11.567	-7.637	18.707		28.78
ATOM	1169	CA	MET	1637	12.107	-6.539	17.927		27.29
MOTA	1170	CB	MET	1637	13.325	-7.008.	17.138		27.97
ATOM	1171	CG	MET	1637	14.446	-7.576	17.982		29.31
ATOM	1172	SD	MET	1637	15.051	-6.440	19.245		29.58
ATOM	1173	CE	MET	1637	15.163	-7.542	20.648		23.51
ATOM	1174	C	MET	1637	11.033	-6.108	16.951		26.60
ATOM	1175	0	MET	1637	10.479	-6.951	16.244		26.60
ATOM	1176	N	LYS	1638	10.758	-4.805	16.893		24.35
ATOM	1177	CA	LYS	1638	9.745	-4.255	16.006		20.79
ATOM	1178	CB	LYS	1638	8.495	-3.883	16.793		18.95
ATOM	1179	CG	LYS	1638	7.723	-5.087	17.268		22.82
ATOM	1180	CD	LYS	1638	6.442	-4.699	17.969	1.00	25.49
MOTA	1181	CE	LYS	1638	5.560	-5.934	18.189	1.00	24.36
ATOM	1182	NZ	LYS	1638	4.892	-6.414	16.941	1.00	22.23
MOTA	1183	С	LYS	1638	10.254	-3.034	15.257	1.00	22.79
ATOM	1184	0	LYS	1638	10.613	-2.041	15.868	1.00	24.60
MOTA	1185	N	ILE	1639	10.259	-3.101	13.934	1.00	23.92
MOTA	1186	CA	ILE	1639	10.707	-1.984	13.113	1.00	24.22
MOTA	1187	CB	ILE	1639	10.925	-2.439	11.648	1.00	
MOTA	1188	CG2		1639	11.270	-1.262	10.766	1.00	
ATOM	1189	CG1	ILE	1639	12.068	-3.454	11.604	1.00	
ATOM	1190	CD1	ILE	1639	11.975	-4.369	10.461		26.92



		1191	C	ILE	1639	0	co.c					
		1192	0	ILE	1639			0.846		173	1.00	25.63
		1193	N	ALA	1640			1.075		042	1.00	26.20
AT	C MO	194		ALA	1640	10.		0.364	13.	390	1.00	27.31
		.195	_	ALA	1640			1.577	13.4	197	1.00	27.45
AT	OM 1	196	_	ALA	1640		523	2.211	14.6		1.00	27.20
ATO	OM 1	197			1640	9.1	720 :	2.595	12.4		1 00	27.20
ATO	OM 1	198				10.7		2.522	11.7		1 00	26.95
ATO		199			1641	8.8		3.551	12.2		1 00	20.95
ATO		200			1641	8.9		.631	11.2		1.00	29.66
ATC		201			1641	10.0		5.581	11.6		1.00	31.25
ATC		202	_	_	1641	9.7		.551	12.7			33.40
ATO		203	OD1 A		1641	10.4		. 524	12.9		00	33.86
ATO		204	OD2 A		1641	8.6		.355	13.4		00	37.57
ATO		205			641	9.0		.228			. 00	29.83
ATO					641	9.5	_	.022	9.79	_		30.77
ATO			_		642	8.63		.032	8.96			29.52
ATO					642	8.66		. 528	9.47		.00	30.38
ATOM				HE 1	642	8.45		.009	8.11		.00 2	29.43
ATON				IE 1	642	7.16			8.10		.00 2	25.46
	<del>-</del>		CD1 PF		642	6.00		555	8.69		.00 2	0.44
ATOM			CD2 PF		542	7.11		547	7.94		.00 2	2.76
ATOM			CE1 PH		542	4.79			10.00	7 1.	00 1	8.52
ATOM			CE2 PH	E 16	542	5.92			8.48	51.	00 2	5.55
ATOM	_		Z PH	_	42			341	10.55	91.	00 2	1.76
ATOM		.5 C	PH		42	4.76			9.80	21.	00 2	4.94
ATOM			PH		42	7.68	_	242	7.16	3 1.	00 3:	1.03
ATOM		.7 N			43	7.946		330	5.975	5 1.	00 39	5.19
ATOM	121	8 C			43	6.600		791	7.693	1.	00 30	1 42
ATOM	121	9 0				5.640		476	6.845	1.6	00 28	. 27
ATOM	122	0 0				5.736	-	991	6.874	1.0	00 28	1 46
ATOM	122	1 N				4.896		707	6.332		00 24	. 20
ATOM	122	2 C2				6.816		171	7.458	1.0	00 31	65
ATOM	122					7.077			7.601	-	0 36	.03
ATOM	1224					8.363			8.389		0 32	47
ATOM	1225		1 LEU			8.321	9.1	~ —	9.446		0 35	·#T
ATOM	1226					7.161	8.8		0.384	1.0	0 37	.30
ATOM	1227					9.663	9.1		0.190	1 0	0 3/	. 60
ATOM	1228		LEU			7.178	8.7		5.293	1.0	0 36	. 62
ATOM	1229		LEU	164		7.770	8.26		5.312	1.0	0 40.	.21
ATOM	1230		ALA	164		6.553	9.88		.293	1.0	0 40.	. 65
ATOM	1231	CB		164		6.591	10.78		.148	1.0	0 44.	50
ATOM	1232	C		164		5.432	11.76		.241	1.00	0 48.	66
ATOM	1233		ALA	164		7.935	11.54		.173	1.00	9 45.	63
ATOM		0	ALA	164		8.254	12.20		.163	1.00	51.	32
ATOM	1234	N	ALA	164	5	8.727	11.44			1.00	52.	68
ATOM	1235	CA	ALA	1646	5	10.023	12.12		.107	1.00	52.	77
	1236	CB	ALA	1646		11.108	11.19		.077	1.00	54.	73
ATOM	1237	C	ALA	1646	5	10.446	12.60		. 646	1.00	55.	34
ATOM	1238	0	ALA	1646		10.430			. 692	1.00	56.4	41
ATOM	1239	N	ASP	1647		10.811	11.82		740	1.00	57.	76
ATOM	1240	CA	ASP	1647		11.280	13.876		567	1.00	58.2	20
ATOM	1241	CB	ASP	1647		10.898	14.394		283	1.00	59.3	19
MOTA	1242	CG	ASP	1647			15.861		083	1.00	59.2	9
						11.128	16.339	→ -0.	356	1.00	60.6	7
											_	

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ATOM	1243	OD1	ASP	1647	12.110	15.908	-1.009	1.00	61.21
MOTA	1244	OD2	ASP	1647	10.337	17.173	-0.835	1.00	61.34
ATOM	1245	C	ASP	1647	12.793	14.236	1.273	1.00	60.16
ATOM	1246	0	ASP	1647	13.523	15.023	1.889	1.00	58.16
MOTA	1247	N	ILE	1648	13.248	13.209	0.562	1.00	61.28
ATOM	1248	CA	ILE	1648	14.658	12.878	0.439	1.00	62.12
ATOM	1249	СВ	ILE	1648	14.848	11.626	-0.444		59.97
ATOM	1250	CG2	ILE	1648	14.023	10.469	0.131	1.00	58.26
ATOM	1251	CG1	ILE	1648	14.429	11.922	-1.883	1.00	55.69
ATOM	1252	CD1	ILE	1648	15.005	10.976	-2.890	1.00	54.38
ATOM	1253	С	ILE	1648	15.470	14.047	-0.127	1.00	65.02
MOTA	1254	0	ILE	1648	16.633	14.245	0.233		66.85
MOTA	1255	N	HIS	1649	14.844	14.839	-0.995		65.85
ATOM	1256	CA	HIS	1649	15.505	15.992	-1.589		66.73
MOTA	1257	CB	HIS	1649	14.859	16.358	-2.934		65.67
MOTA	1258	CG	HIS	1649	15.142	15.388	-4.038		66.47
ATOM	1259	CD2	HIS	1649	16.253	14.686	-4.355		67.11
ATOM	1260	ND1	HIS	1649	14.210	15.064	-4.999	1.00	65.21
ATOM	1261	CE1	HIS	1649	14.733	14.216	-5.867		66.52
ATOM	1262	NE2	HIS	1649	15.974	13.966	-5.494	1.00	66.25
MOTA	1263	C	HIS	1649	15.505	17.200	-0.663	1.00	68.55
MOTA	1264	0	HIS	1649	15.636	18.341	-1.116	1.00	69.35
ATOM	1265	N	HIS	1650	15.273	16.963	0.629		71.25
ATOM	1266	CA	HIS	1650	15.262	18.026	1.633		73.53
ATOM	1267	CB	HIS	1650	13.849	18.551	1.860	1.00	76.79
MOTA	1268	CG	HIS	1650	13.342	19.448	0.765		83.36
ATOM	1269	CD2	HIS	1650	13.509	20.772	0.537	1.00	86.47
ATOM	1270	ND1	HIS	1650	12.571	18.984	-0.270	1.00	87.02
ATOM	1271	CEl	HIS	1650	12.279	19.983	-1.076	1.00	88.66
MOTA	1272	NE2	HIS	1650	12.840	21.080	-0.609	1.00	88.34
MOTA	1273	С	HIS	1650	15.872	17.580	2.965	1.00	73.11
MOTA	1274	0	HIS	1650	15.686	18.241	3.977	1.00	73.23
MOTA	1275	N	ILE	1651	16.599	16.464	2.949	1.00	72.64
ATOM	1276	CA	ILE	1651	17.234	15.937	4.143	1.00	72.54
ATOM	1277	CB	ILE	1651	17.660	14.472	3.942	1.00	74.59
ATOM	1278	CG2	ILE	1651	18.463	13.966	5.142	1.00	75.52
ATOM	1279	CG1	ILE	1651	16.426	13.591	3.752	1.00	77.59
ATOM	1280	CD1	ILE	1651	16.747	12.141	3.472	1.00	
MOTA	1281	С	ILE	1651	18.463	16.769	4.523	1.00	71.47
ATOM	1282	0	ILE	1651	19.326	17.022	3.688	1.00	72.40
ATOM	1283	N	ASP	1652	18.529	17.197	5.784	1.00	70.34
ATOM	1284	CA	ASP	1652	19.678	17.976	6.235	1.00	68.57
ATOM	1285	CB	ASP	1652	19.272	18.878	7.411	1.00	72.80
ATOM	1286	CG	ASP	1652	20.456	19.640	7.982	1.00	76.90
ATOM	1287	OD1		1652	21.463	19.888	7.287	1.00	79.62
ATOM	1288	OD2		1652	20.369	20.030	9.170	1.00	80.36
ATOM	1289	С	ASP	1652	20.771	17.007	6.652	1.00	66.01
ATOM	1290	0	ASP	1652	20.709	16.421	7.735	1.00	
ATOM	1291	N	TYR	1653	21.778	16.868	5.808	1.00	64.05
ATOM	1292	CA	TYR	1653	22.906	15.978	6.074	1.00	63.55
ATOM	1293	CB	TYR	1653	23.829	15.913	4.855	1.00	63.81
ATOM	1294	CG	TYR	1653	23.316	14.993	3.771	1.00	65.65

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An	OM 129	5 CD1 TYR	1653					
	OM 129	6 CE1 TYR		24.0			643 1.00	65.32
	OM 129	7 CD2 TYR		23.6			674 1.00	68.40
AT			1653	22.0			903 1.00	66.72
AT			1653	21.6		151 2.9		69.93
AT		OH TYR	1653	22.4	_	1.82		70.13
AT			1653	21.96			02 1.00	72.73
ATO			1653	23.70	_		28 1.00	62.96
ATO			1654	24.34			38 1.00	63.31
ATO	,	CA TYR	1654	23.65			27 1.00	63.02
ATC		CB TYR	1654	24.37			02 1.00	63.89
ATO		CG TYR	1654	24.89		91 8.6		60.37
ATO		CD1 TYR	1654	26.01		65 7.6		59 33
ATO		CE1 TYR	1654	25.73	-	73 6.33		59.29
ATO		CD2 TYR	1654	26.75		37 5.36	1.00	51 50
ATO		CE2 TYR	1654	27.349	_	30 8.0 <i>6</i>		50 05
ATO		CZ TYR	1654	28.384	_	8 7.11		50.05 51.3E
ATOM		OH TYR	1654	28.082	-	8 5.77		2 41
ATON	1 1313	C TYR	1654	29.098		9 4.84		O E2
ATOM	1 1314		1654	23.586		4 10.19		5 65
ATOM		17	1655	24.104	_	1 11.25		7 21
ATOM	1316	~	1655	22.349		4 10.11		7.51
ATOM	1317	<b>6</b> 5	16 <b>5</b> 5	21.499	-	0 11.30		/.JZ
ATOM	1318	GG	1655	20.028		5 10.89		3.54 1 / 0
ATOM	1319	CD -	L655	19.057		12.049		3 00
ATOM	1320		1655	17.648	17.713	11.531		5 55
ATOM	1321		.655	16.624	17.320	12.568		0.73
ATOM	1322		.655	15.232	17.521	12.072		5.54
ATOM	1323		655	21.783	16.102	12.076		
ATOM	1324		656	21.952	15.032	11.478		.43
ATOM	1325		656	21.825	16.218			.11
ATOM	1326		656	22.093	15.079	14.274		.03
ATOM	1327	aa	656	23.049	15.481	15.394	1.00 67	72
ATOM	1328 (		556	24.473	15.716	14.947	1.00 66	.34
ATOM	1329 (	TP 7.00	556	25.326	16.124	16.136	1.00 66	.60
ATOM	1330 h	TP	556	26.801	15.839	15.905	1.00 64	. 71
ATOM	1331 (		556	27.612	16.059	17.138	1.00 62	.24
ATOM	1332 (		56	20.823	14.480	14.881	1.00 70.	67
ATOM	1333 V		57	19.759	15.104	14.864	1.00 71.	91
ATOM	1334 C		57	20.941	13.265	15.412	1.00 69.	38
ATOM			57	19.818 20.052	12.586	16.035	1.00 68.	30
ATOM	1336 O	C	57		11.051	16.101	1.00 69.	30
ATOM	1337 C	G2 THR 16		_	10.757	16.941	1.00 68.	20
ATOM	1338 C				10.479	14.713	1.00 69.	71
ATOM	1339 0			19.706	13.145	17.445	1.00 67.	60
MOTA	1340 N				13.971	17.846	1.00 67.	40
ATOM	1341 C				12.694	18.206	1.00 67.8	33
ATOM	1342 CE				13.163	19.582	1.00 67.	73
ATOM	1343 C	ALA 165		17.345	12.503	20.234	1.00 68.8	37
ATOM	1344 O	ALA 165		19.833	12.820	20.364	1.00 66.5	9
ATOM	1345 N	ASN 165		20.368 1	13.640	21.115	1.00 66.3	3
ATOM	1346 CA				1.616	20.129	1.00 65.3	8
			-	21.545 1	1.143	20.801	1.00 62.6	5
							0	_

ATOM	1347	CB	ASN	1659	21.702	9.638	20.616	1.00	63.61
ATOM	1348	CG	ASN	1659	22.548	9.009	21.697		64.09
ATOM	1349	OD1		1659	22.526	9.451	22.850	1.00	63.69
ATOM	1350	ND2	ASN	1659	23.279	7.959	21.345	1.00	64.10
MOTA	1351	С	ASN	1659	22.808	11.844	20.321	1.00	60.46
ATOM	1352	0	ASN	1659	23.882	11.601	20.856	1.00	60.78
MOTA	1353	N	GLY	1660	22.671	12.675	19.285	1.00	58.84
ATOM	1354	CA	GLY	1660	23.803	13.407	18.735	1.00	56.69
ATOM	1355	С	GLY	1660	24.570	12.721	17.616	1.00	56.40
ATOM	1356	0	GLY	1660	<b>25.7</b> 38	13.028	17.377	1.00	56.43
MOTA	1357	N	ARG	1661	23.929	11.779	16.937	1.00	56.00
ATOM	1358	CA	ARG	1661	24.585	11.048	15.849	1.00	53.80
ATOM	1359	CB	ARG	1661	24.312	9.540	15.952	1.00	54.52
MOTA	1360	CG	ARG	1661	24.876	8.879	17.218	1.00	55.28
MOTA	1361	CD	ARG	1661	24.556	7.395	17.226	1.00	58.01
ATOM	1362	NE	ARG	1661	25.051	6.670	18.396	1.00	58.41
ATOM	1363	CZ	ARG	1661	24.918	5.355	18.559	1.00	59.08
MOTA	1364	NH1	ARG	1661	24.306	4.637	17.623	1.00	55.82
MOTA	1365	NH2	ARG	1661	25.394	4.762	19.652	1.00	57.53
MOTA	1366	C	ARG	1661	24.139	11.581	14.491	1.00	51.03
MOTA	1367	0	ARG	1661	23.160	12.323	14.401	1.00	48.69
MOTA	1368	N	LEU	1662	24.859	11.189	13.440	1.00	48.33
MOTA	1369	CA	LEU	1662	24.565	11.647	12.087	1.00	45.87
ATOM	1370	CB	LEU	1662	25.839	12.199	11.426	1.00	46.18
ATOM	1371	CG	LEU	1662	26.374	13.511	12.016	1.00	45.78
MOTA	1372	CD1	LEU	1662	27.856	13.681	11.722	1.00	45.92
MOTA	1373	CD2	LEU	1662	25.576	14.698	11.489	1.00	44.92
ATOM	1374	С	LEU	1662	23.961	10.542	11.230	1.00	43.02
MOTA	1375	O	LEU	1662	24.647	9.607	10.811	1.00	42.04
MOTA	1376	N	PRO	1663	22.648	10.640	10.968	1.00	41.48
ATOM	1377	CD	PRO	1663	21.769	11.718	11.468	1.00	40.54
MOTA	1378	CA	PRO	1663	21.886	9.680	10.161	1.00	39.60
ATOM	1379	CB	PRO	1663	20.582	10.424	9.889	1.00	38.77
ATOM	1380	CG	PRO	1663	20.386	11.183	11.151	1.00	40.83
ATOM	1381	С	PRO	1663	22.578	9.273	8.860		35.90
ATOM	1382	0	PRO	1663	22.448	8.124	8.427		36.85
ATOM	1383	N	VAL	1664	23.356	10.180	8.276		33.16
ATOM	1384	CA	VAL	1664	24.053	9.880	7.024		32.51
MOTA	1385	СВ	VAL	1664	24.851	11.106	6.439		32.44
ATOM	1386	CG1		1664	23.917	12.213	6.065		26.99
ATOM	1387	CG2		1664	25.897	11.607	7.421		29.84
ATOM	1388	С	VAL	1664	24.989	8.675	7.158		30.30
MOTA	1389	0	VAL	1664	25.400	8.091	6.161		30.16
ATOM	1390	N	LYS	1665	25.278	8.276	B.393		27.72
MOTA	1391	CA	LYS	1665	26.170	7.151	8.649		27.96
ATOM	1392	CB	LYS	1665	26.808	7.276	10.025		26.42
ATOM	1393	CG	LYS	1665	27.857	8.351	10.061		28.20
ATOM	1394	CD	LYS	1665	28.221	8.754	11.478		32.47
ATOM	1395	CE	LYS	1665	29.398	9.720	11.468		32.33
ATOM	1396	NZ	LYS	1665	29.713	10.231	12.819		30.38
MOTA	1397	С	LYS	1665	25.522	5.794	8.486		25.81
ATOM	1398	0	LYS	1665	26.159	4.769	8.691	1.00	27.53

דימ	OM 1	300										
		399	N	TRP	1666	24.	247	5.7	792 0			
AT		400	CA	TRP	1666		499	4.5		120	1.00	26.13
AT		401		TRP	1666	22.		4.5		896	1.00	25.88
		402		TRP	1666	22.	547			800	1.00	26.15
AT	~	103	CD2	TRP	1666	23.		4.0			1.00	28.12
ATO		104	CE2	rrp	1666	23.		4.8			1.00	26.14
ATO		105	CE3	rp	1666	23.3		4.0	•		1.00	24.97
ATO		06	CD1	rrp	1666			6.2			1.00	25.14
ATC	DM 14	07	NE1	RP	1666	22.4		2.7				26.09
ATC		08		RP	1666	22.7		2.7	51 12.0	34	1.00	22.55
ATC	)M 14	09		'RP	1666	23.6		4.45	53 13.6	84	1.00	25.32
ATO			_	'RP		23.7		6.66	54 12.7	12	1.00	21.72
ATO	M 14			RP	1666	23.9		5.78	32 13.7		1 00	23.77
ATO				RP	1666	23.0		4.44	4 6.4		1 00	23.77 24.79
ATO			_	et Et	1666	22.6		3.39			1 00	24.79
ATO					1667	23.3	50	5.50			1.00	25.26
ATO					1667	22.96	53	5.56	•		1.00	24.21
ATON				_	1667	22.79	96	7.01			1.00	23.79
ATON		_			1667	21.79		7.81			1.00	25.08
ATOM		_	SD MI	T	1667	21.77		9.49			1.00 3	32.58
ATOM			E MI	T	1667	21.01		9.20	_		.00 4	11.43
ATOM		_		T :	1667	23.93		4.942			00 4	0.85
		-	ME	T :	1667	25.13					.00 2	2.52
ATOM				_	1668	23.40		5.173			.00 2	3.63
ATOM		_	A AL	A ]	1668	24.21		4.195			.00 2	2.77
ATOM		3 C	B AL		.668	23.34		3.576			.00 2	4.91
ATOM		_	AL		668		_	2.672		6 1	.00 2	4.41
ATOM		5 0	AL		668	24.80		4.706		8 1	.00 2	6.66
ATOM	1426	5 N	PR		669	24.163		5.748		1 1	.00 2	4.54
ATOM	1427	CI	PR		669	26.013		4.511	-0.10	1 1.	.00 26	5.97
ATOM	1428	C.	PRO		669	26.935		3.374	0.066	5 1.	.00 26	5.23
ATOM	1429	CE			669	26.614		5.563	-0.919	9 1.	00 26	5.05
ATOM	1430	CG		_	669	27.855		.876	-1.482	2 1.	00 24	1.03
ATOM	1431	C	PRO	_	669	28.259		.946	-0.358	1.	00 26	27
ATOM	1432	0	PRO			25.687		.048	-2.030		00 26	44
ATOM	1433	N	GLU		569	25.576		.250	-2.263		00 27	77
ATOM	1434	CA			70	24.971		.137	-2.685		00 27	. 12
ATOM	1435	CB			70	24.093		. 553	-3.769		00 27	. 10
ATOM	1436	CG		-	70	23.613		.365	-4.614		00 27	.63
ATOM	1437	CD	GLU		70	22.545		. 492	-3.980		00 29	. 35
ATOM	1438		GLU		70	23.089		. 238	-3.310		00 29	
ATOM	1439	OE:			70	22.248		430	-2.874	1.0	00 28	. 03
ATOM			GLU	16		24.325		040	-3.215	1.(	00 24	. 12
ATOM	1440	C	GLU	16	70	22.931		407		1.0	00 26.	. 07
	1441	0	GLU	16	70	22.477		281	-3.301	1.0	0 25.	52
ATOM	1442	N	ALA	16	71	22.452			-4.042	1.0	0 24.	12
ATOM	1443	CA	ALA	16	71	21.337		163	-2.084	1.0	0 27.	74
ATOM	1444	CB	ALA	16		20.729		928	-1.510	1.0	0 27.	65
ATOM	1445	С	ALA	167		21.860		189	-0.319	1.0	0 23.	18
ATOM	1446	0	ALA	167				283	-1.065	1.0	0 28.	22
ATOM	1447	N	LEU	167		21.234		310	-1.305	1.0	0 28.	51
ATOM	1448	CA	LEU	167		23.011		266	-0.406	1.0	0 30.	60
ATOM	1449	СВ	LEU	167		23.647		484	0.074	1.0	0 32.	67
ATOM	1450	CG	LEU			24.831		127	0.952	1.00	0 32.	05
		-		167	4	25.662	10.	264	1.527	1.00	34.0	20

т пом	1451	an.	* ***	1670	04 034	10 001			
ATOM	1451		LEU	1672	24.874	10.981	2.577	1.00 3	
ATOM	1452		LEU	1672	26.910	9.667	2.149		5.22
ATOM	1453	C	LEU	1672	24.121	10.398	-1.067		7.10
ATOM	1454	0	LEU	1672	23.799	11.580	-1.086	1.00 3	
MOTA	1455	N	PHE	1673	24.905	9.858	-1.997	1.00 3	
MOTA	1456	CA	PHE	1673	25.403	10.664	-3.102	1.00 3	
ATOM	1457	CB	PHE	1673	26.692	10.061	-3.667	1.00 3	
ATOM	1458	CG	PHE	1673	27.782	9.857	-2.644	1.00 3	
ATOM	1459	CD1		1673	28.456	8.633	-2.566	1.00 3	
ATOM	1460	CD2		1673	28.143	10.874	-1.762	1.00 3	
ATOM	1461	CE1		1673	29.467	8.421	-1.623	1.00 3	4.66
ATOM	1462	CE2		1673	29.156	10.678	-0.816	1.00 3	
ATOM	1463	CZ	PHE	1673	29.819	9.444	-0.748		4.81
MOTA	1464	C	PHE	1673	24.406	10.890	-4.245	1.00 3	9.03
ATOM	1465	0	PHE	1673	24.276	11.997	-4.734	1.00 3	9.02
ATOM	1466	N	ASP	1674	23.693	9.844	-4.651	1.00 4	
MOTA	1467	CA	ASP	1674	22.757	9.931	-5.762	1.00 4	
MOTA	1468	CB	ASP	1674	22.957	8.736	-6.700	1.00 4	6.08
ATOM	1469	CG	ASP	1674	24.384	8.617	-7.201	1.00 5	1.20
MOTA	1470		ASP	1674	25.057	9.663	-7.333	1.00 5	3.97
MOTA	1471		ASP	1674	24.822	7.470	-7. <b>4</b> 69	1.00 5	0.65
ATOM	1472	С	ASP	1674	21.263	9.999	-5.418	1.00 4	2.89
ATOM	1473	0	ASP	1674	20.427	10.079	-6.317	1.00 4	1.95
ATOM	1474	N	ARG	1675	20.923	9.899	-4.134	1.00 4	2.82
MOTA	1475	CA	ARG	1675	19.521	9.944	-3.706	1.00 4	2.64
ATOM	1476	CB	ARG	1675	18.890	11.300	-4.028	1.00 4	3.80
ATOM	1477	CG	ARG	1675	19.480	12.449	-3.252	1.00 6	1.19
ATOM	1478	CD	ARG	1675	19.407	13.727	-4.068	1.00 7	2.90
ATOM	1479	NE	ARG	1675	20.025	14.854	-3.381	1.00 8	3.15
MOTA	1480	CZ	ARG	1675	19.652	16.123	-3.539	1.00 88	3.21
ATOM	1481	NHl		1675	18.662	16.439	-4.365	1.00 8	9.58
MOTA	1482	NH2	ARG	1675	20.265	17.085	-2.860	1.00 92	2.07
ATOM	1483	C	ARG	1675	18.674	8.825	-4.299	1.00 38	3.05
MOTA	1484	0	ARG	1675	17.495	9.005	-4.588	1.00 38	3.87
MOTA	1485	N	ILE	1676	19.281	7.658	-4.479	1.00 34	1.44
ATOM	1486	CA	ILE	1676	18.576	6.514	-5.012	1.00 30	).11
ATOM	1487	CB	ILE	1676	19.378	5.825	-6.096	1.00 29	€.58
ATOM	1488	CG2	ILE	1676	18.509	4.850	-6.797	1.00 30	0.72
MOTA	1489	CG1		1676	19.835	6.868	-7.116	1.00 34	1.29
ATOM	1490		ILE	1676	20.798	6.348	-8.145	1.00 41	1.15
ATOM	1491	C	ILE	1676	18.315	5.541	-3.874	1.00 26	5.90
ATOM	1492	0	ILE	1676	19.236	4.898	-3.364	1.00 22	2.06
ATOM	1493	N	TYR	1677	17.056	5.465	-3.454	1.00 28	3.17
ATOM	1494	CA	TYR	1677	16.677	4.589	-2.350	1.00 26	.80
MOTA	1495	CB	TYR	1677	15.742	5.310	-1.398	1.00 26	.05
ATOM	1496	CG	TYR	1677	16.442	6.367	-0.580	1.00 26	.92
ATOM	1497		TYR	1677	16.510	7.693	-1.018	1.00 23	.98
ATOM	1498		TYR	1677	17.129	8.665	-0.250	1.00 23	.90
ATOM	1499		TYR	1677	17.022	6.048	0.644	1.00 26	.99
ATOM	1500		TYR	1677	17.642	7.017	1.414	1.00 24	.87
ATOM	1501	CZ	TYR	1677	17.685	8.315	0.968	1.00 26	.44
ATOM	1502	OH	TYR	1677	18.227	9.273	1.783	1.00 30	.89

AT	OM 1505	_		
AT			TYR 1677	16.006 3.350 -2.894 1.00 26 20
ATO			TYR 1677	15 000 3 4 5
		N 7	THR 1678	16 499 2 100 28.12
ATO			THR 1678	15 972 0 25.46
ATO		CB 1	THR 1678	16 904 0 225
ATO	_	OG1 1	HR 1678	18 195 0 207
ATC		CG2 T	HR 1678	17 060 30.59
ATO		C T	HR 1678	15 000 1.305 -5.174 1.00 26.56
ATO		O T	HR 1678	16 476 -0.049 -1.758 1.00 24.60
ATO	<b></b>	N H	IS 1679	10.176 0.277 -0.693 1.00 27 15
ATO		CA H	IS 1679	13.300 -1.260 -1.974 1.00 23 23
ATO			IS 1679	$\frac{13.496}{2.276}$ $-0.933$ $1.00$ 21 51
ATO	M 1515	CG H		$\frac{11.747}{3.520}$ $\frac{-3.520}{-1.411}$ 1.00 20 84
ATO	M 1516	CD2 H	IS 1679	-3.279 -1.695 1.00 21 49
ATON	1 1517	ND1 HI	_	12.552 -3.476 -2.812 1 00 22 22
ATON		CE1 HI		12.423 -2.795 -0.741 1.00 00 00
ATOM		NE2 HI		11.206 -2.713 -1.255 1 00 30 55
ATOM		C HI		11.255 -3.116 -2.515 1 00 22.60
ATOM		_		16 976 2 500
ATOM				17 350 2 051
ATOM				17 799 2 300
ATOM		CA GL		19 249 2 507
ATOM		CB GL		19 860 2 455
ATOM		CG GLI		19 896 2 575
ATOM	-	D GL		19 015 3 550
ATOM		E1 GL		18 069 2 202 1.00 37.77
ATOM		E2 GLN	•	19 321 4 355
ATOM	1529 C			19 913 1 600
ATOM	1530 O			20 814 7 00-
ATOM	1531 N			19 514 0 221 1.00 21.53
ATOM	1532 C		1681	20 129 0 500
ATOM	1533 C		1681	19 841 2 255
ATOM	1534 0	G SER	1681	18 472 2 22"
ATOM	1535 C	SER	1681	19 695 0 200
ATOM	1536 O	SER	1681	20 457 0 513 1.00 23.91
	1537 N	ASP	1682	18 511 0 700 26.70
ATOM	1538 C	ASP	1682	18 044
ATOM	1539 CE	ASP	1682	16 505 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7
ATOM	1540 CG		1682	15 560 0 000
ATOM	1541 OD	1 ASP	1682	14 363 0 000
ATOM		2 ASP	1682	15 949 1 100 21.99
ATOM	1543 C	ASP	1682	19 055 1 3.436 1.00 24.42
ATOM	1544 O	ASP	1682	19 290 3.011 1.00 20.86
ATOM	1545 N	VAL	1683	19 202 -1.770 4.799 1.00 21.62
ATOM	1546 CA	VAL	1683	20.336 -2.649 2.727 1.00 21.60
ATOM	1547 CB	VAL	1683	30.507 -3.732 3.122 1.00 22.27
ATOM	1548 CG:	l VAL	1683	20.315 -4.740 1.965 1.00 22.22
ATOM		2 VAL	1683	2.315 1.00 21.52
ATOM	1550 C	VAL	1683	19.187 -5.437 1.662 1.00 20.89
ATOM	1551 O	VAL	1683	21.010 -3.150 3.666 1.00 21 96
ATOM	1552 N	TRP	1684	22.107 -3.577 4.705 1.00 24 39
ATOM	1553 CA	TRP		22.172 -2.160 2.970 1.00 22 01
ATOM	1554 CB	TRP	1684	23.375 -1.489 3.449 1.00 27.05
	- 25	ANE	1684	23.685 -0.273 2.566 1.00 20.25
				20.25

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MOTA	1555	CG	TRP	1684	24.808	0.549	3.069	1.00 22.35
MOTA	1556		TRP	1684	26.118	0.644	2.503	1.00 24.14
ATOM	1557		TRP	1684	26.879	1.500	3.334	1.00 23.68
ATOM	1558	CE3		1684	26.728	0.091	1.370	1.00 25.09
ATOM	1559	CD1		1684	24.825	1.346	4.193	1.00 22.52
ATOM	1560	NE1	TRP	1684	26.066	1.915	4.355	1.00 21.48
ATOM	1561	CZ2	TRP	1684	28.216	1.815	3.061	1.00 20.56
MOTA	1562	CZ3	TRP	1684	28.059	0.405	1.095	1.00 23.92
MOTA	1563	CH2	TRP	1684	28.785	1.257	1.942	1.00 23.18
MOTA	1564	С	TRP	1684	23.105	-1.025	4.903	1.00 23.96
ATOM	1565	0	TRP	1684	23.889	-1.308	5.815	1.00 25.98
MOTA	1566	N	SER	1685	21.992	-0.332	5.118	1.00 24.68
ATOM	1567	CA	SER	1685	21.615	0.144	6.447	1.00 22.75
ATOM	1568	СВ	SER	1685	20.266	0.870	6.376	1.00 21.11
ATOM	1569	OG	SER	1685	20.276	1.950	5.452	1.00 21.98
ATOM	1570	С	SER	1685	21.516	-1.011	7.457	1.00 23.06
MOTA	1571	0	SER	1685	21.865	-0.850	8.638	1.00 22.55
ATOM	1572	N	PHE	1686	21.041	-2.168	6.998	1.00 21.83
ATOM	1573	CA	PHE	1686	20.915	-3.340	7.854	1.00 21.92
ATOM	1574	CB	PHE	1686	20.153	-4.457	7.129	1.00 18.02
MOTA	1575	CG	PHE	1686	19.965	-5.683	7.971	1.00 20.86
MOTA	1576		PHE	1686	19.142	-5.641	9.108	1.00 18.76
ATOM	1577		PHE	1686	20.669	-6.853	7.688	1.00 18.96
ATOM	1578		PHE	1686	19.023	-6.743	9.947	1.00 19.29
ATOM	1579		PHE	1686	20.554	-7.965	8.514	1.00 19.27
ATOM	1580	CZ	PHE	1686	19.732	-7.908	9.653	1.00 21.91
ATOM	1581	C	PHE	1686	22.304	-3.845	8.316	1.00 22.11
ATOM	1582	0	PHE	1686	22.473	-4.378	9.436	1.00 21.35
MOTA	1583	N	GLY	1687	23.294	-3.691	7.436	1.00 20.48
MOTA	1584	CA	GLY	1687	24.653	-4.079	7.769	1.00 20.41
MOTA	1585	С	GLY	1687	25.185	-3.211	8.899	1.00 19.03
MOTA	1586	0	GLY	1687	25.857	-3.714	9.808	1.00 20.27
MOTA	1587	N	VAL	1688	24.893	-1.906	8.829	1.00 20.57
ATOM	1588	CA	VAL	1688	25.296	-0.937	9.860	1.00 21.14
MOTA	1589	CB	VAL	1688	24.974	0.548	9.467	1.00 20.78
MOTA	1590	CG1		1688	25.440	1.493	10.564	1.00 21.51
ATOM	1591	CG2		1688	25.681	0.923	8.186	1.00 19.70
ATOM	1592	C	VAL	1688	24.547	-1.297	11.142	1.00 23.16
ATOM	1593	0	VAL	1688	25.126	-1.271	12.225	1.00 24.14
ATOM	1594	N	LEU	1689	23.264	-1.648	11.021	1.00 24.50
MOTA	1595	CA	LEU	1689	22.465	-2.058	12.187	1.00 25.93
ATOM	1596	CB	LEU	1689	21.008	-2.316	11.776	1.00 25.42
ATOM	1597	CG	LEU	1689	19.933	-2.392	12.874	1.00 26.29
ATOM	1598	CD1		1689	18.572	-2.053	12.272	1.00 23.43
ATOM	1599	CD2		1689	19.885	-3.768	13.543	1.00 25.66
ATOM	1600	С	LEU	1689	23.080	-3.330	12.797	1.00 28.01
ATOM	1601	0	LEU	1689	23.203	-3.426	14.016	1.00 30.06
ATOM	1602	N	LEU	1690	23.487	-4.287	11.956	1.00 27.19
ATOM	1603	CA	LEU	1690	24.111	-5.520	12.457	1.00 25.29
ATOM	1604	CB	LEU	1690	24.556	-6.446	11.315	1.00 24.98
ATOM	1605	CG	LEU	1690	23.594	-7.390	10.589	1.00 24.85
MOTA	1606	CD1	LEU	1690	24.385	-8.132	9.538	1.00 24.22

ATO	-00,	CD2	LEU 1690	20
ATC			EU 1690	22.300 -8.434 11.512 1.00 10 10
ATC		_	EU 1690	25.326 -5.123 13.291 1.00 24 70
OTA	M 1610		'RP 1691	25.521 -5.624 14.408 1 00 27 57
ATO	M 1611			26.117 -4.197 12 747 1 00
ATO			RP 1691 RP 1691	27.316 -3.693 13.425 1.00 23.68
ATO	M 1613	_		27.998 -2.621 12 567 1 20
ATO!	M 1614	CD2 T		29.331 -2.173 13 105 1 2
MOTA	1 1615			29.565 -1.082 14.004
ATOM	1 1616			30.966
ATOM			RP 1691	28.726 -0.167
ATOM			-051	30.570 -2.700
ATOM		NE1 TE		31.550 -1.00 24.44
ATOM		CZ2 TR		31.543 -0.000
ATOM		CZ3 TR		29.300 0 300 15.034 1.00 24.39
MOTA		CH2 TR		30.700 0.050 15.484 1.00 21.99
ATOM	1622	C TR		26.998 3.13
ATOM	1623	O TR	P 1691	27 772 14.823 1.00 25.87
ATOM	1624	N GL	J 1692	35.301 15.750 1.00 27.39
	1625	CA GL	J 1692	25 450 2.448 14.956 1.00 26.45
ATOM	1626	CB GLU		24 257 16.238 1.00 25.13
ATOM	1627	CG GLt		24 25- 0.933 16.068 1.00 23 56
ATOM	1628	CD GLU		0.091 14.962 1 00 10 73
ATOM	1629	OE1 GLU	1692	23.111 0.935 14 990 7 00
ATOM		DE2 GLU		22.303 0.722 13 962
ATOM	1631 (	GLU		22.919 1.819 15.738 1 00 25 62
ATOM	1632 (			25.072 -2.963 17 225
ATOM	1633 N			<sup>23.2</sup> /8 -2.818 18 422 1
ATOM	1	A ILE	1693	24.484 -4.046 16 720 1 22
ATOM			1693	24.080 -5.164 17.565 1.00 -5.23
ATOM		B ILE G2 ILE	1693	23 177 6 202
ATOM	_	G1 ILE	1693	22.966 -7 465 - 2.00 22.99
ATOM	_	D1 ILE	1693	21 820 5 550
ATOM	1639 C		1693	20.964 -6 305 2.00 20.23
ATOM	3646	ILE	1693	25.322 5.043 1.00 13.67
ATOM	3 - 4 - 1	ILE	1693	25,401 6 106
ATOM		PHE	1694	26.329 -6.053
ATOM			1694	27.503 -6.700 1.00 27.59
ATOM			1694	28.122 -7.622 -7.00 29.42
ATOM	1644 CG		1694	27.142 -9.542 -10.771 1.00 29.37
ATOM		1 PHE	1694	26.522 425 1.00 27.99
3		2 PHE	1694	26.751 0 700
<b>-</b>	1647 CE	1 PHE	1694	25 525 2 17.074 1.00 27.86
	1648 CE	2 PHE	1694	25 753 -3.335 14.625 1.00 30.12
	1649 CZ	PHE	1694	25 126 10.366 16.674 1.00 25.78
	1650 C		1694	28 405 15.453 1.00 26.17
3	1651 O		1694	3.821 18.578 1 00 29 02
3	1652 N		1695	38 317 19.126 1.00 32.81
	1653 CA		1695	18.635 1 00 29 75
ATOM 1	654 CB		1695	29.044 -3.598 19.419 1.00 25 30
ATOM 1			L695	29.540 -2.379 18.627 1.00 21 81
ATOM 1	656 CG2			28.422 -1.628 18.137 1 00 21 54
ATOM 1	657 C	_	695	30.457 -2.816 17 508 1 00 21.54
B Phone	658 O		.695	28.198 -3.126 20.504 1 55
		T1114 1	695	28 620 2 200
				21.386 1.00 26.77
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ATOM	1659	N	LEU	1696	27.023	-3.747	20.747	1.00	26.87
ATOM	1660	CA	LEU	1696	26.069	-3.446	21.813	1.00	27.64
MOTA	1661	CB	LEU	1696	26.572	-3.977	23.156	1.00	30.54
ATOM	1662	CG	LEU	1696	26.903	-5.456	23.182	1.00	29.75
ATOM	1663	CD1	LEU	1696	27.448	-5.821	24.546	1.00	32.53
ATOM	1664	CD2	LEU	1696	25.658	-6.234	22.882	1.00	33.79
ATOM	1665	С	LEU	1696	25.727	-1.984	21.946	1.00	25.51
ATOM	1666	0	LEU	1696	25.824	-1.410	23.025	1.00	27.90
ATOM	1667	N	GLY	1697	25.265	-1.395	20.857	1.00	26.48
ATOM	166B	CA	GLY	1697	24.899	0.007	20.859		25.81
ATOM	1669	С	GLY	1697	26.040	0.900	20.452		26.40
ATOM	1670	0	GLY	1697	26.055	2.090	20.760	1.00	29.69
MOTA	1671	N	GLY	1698	27.008	0.330	19.748	1.00	
MOTA	1672	CA	GLY	1698	28.150	1.110	19.314	1.00	
ATOM	1673	C	GLY	1698	27.795	2.186	18.310	1.00	30.13
ATOM	1674	0	GLY	1698	26.896	2.028	17.496	1.00	32.55
ATOM	1675	N	SER	1699	28.520	3.295	18.375	1.00	
MOTA	1676	CA	SER	1699	28.304	4.420	17.491	1.00	32.11
MOTA	1677	CB	SER	1699	28.622	5.714	18.246	1.00	
ATOM	1678	OG	SER	1699	28.578	6.863	17.407	1.00	38.87
ATOM	1679	С	SER	1699	29.203	4.269	16.268	1.00	32.10
ATOM	1680	0	SER	1699	30.408	4.073	16.403	1.00	31.12
ATOM	1681	N	PRO	1700	28.629	4.324	15.062	1.00	32.70
ATOM	1682	CD	PRO	1700	27.204	4.482	14.745	1.00	34.35
MOTA	1683	CA	PRO	1700	29.427	4.192	13.837	1.00	32.25
ATOM	1684	CB	PRO	1700	28.358	4.096	12.736	1.00	32.85
MOTA	1685	CG	PRO	1700	27.101	3.713	13.461	1.00	35.54
ATOM	1686	C	PRO	1700	30.258	5.456	13.651	1.00	31.84
ATOM	1687	0	PRO	1700	29.792	6.550	13.983	1.00	31.56
MOTA	1688	N	TYR	1701	31.487	5.306	13.170	1.00	31.07
ATOM	1689	CA	TYR	1701	32.372	6.441	12.910	1.00	32.41
MOTA	1690	CB	TYR	1701	32.039	7.055	11.537	1.00	32.39
MOTA	1691	CG	TYR	1701	32.088	6.092	10.378	1.00	35.63
MOTA	1692	CD1		1701	30.936	5.807	9.638	1.00	37.94
ATOM	1693	CE1		1701	30.977	4.955	8.535	1.00	40.79
MOTA	1694	CD2		1701	33.293	5.495	9.990	1.00	37.49
ATOM	1695		TYR	1701	33.351	4.646	8.886	1.00 4	41.82
ATOM	1696	CZ	TYR	1701	32.190	4.382	8.160	1.00 4	45.96
MOTA	1697	ОН	TYR	1701	32.251	3.572	7.039	1.00	
MO'TA	1698	C	TYR	1701	32.377	7.559	13.970	1.00	
ATOM	1699	0	TYR	1701	32.066	8.711	13.679	1.00	32.41
ATOM	1700	N	PRO	1702	32.753	7.229	15.215	1.00	
ATOM	1701	CD	PRO	1702	33.288	5.946	15.695	1.00 3	35.64
ATOM	1702	CA	PRO	1702	32.775	8.258	16.270	1.00 3	33.68
ATOM	1703	CB	PRO	1702	33.321	7.499	17.482	1.00 3	32.52
ATOM	1704	CG	PRO	1702	33.063	6.061	17.166	1.00 3	88.81
ATOM	1705	С	PRO	1702	33.736	9.388	15.919	1.00 3	
ATOM	1706	0	PRO	1702	34.875	9.145	15.522	1.00 3	
MOTA	1707	N	GLY	1703	33.275	10.625	16.089	1.00 3	
MOTA	1708		GLY	1703	34.101	11.792	15.802	1.00 3	32.51
ATOM	1709		GLY	1703	34.232	12.166	14.339	1.00 3	
ATOM	1710	0	GLY	1703	34.904	13.146	14.005	1.00 3	11.22

ATC	_	711	N	VAL	1704	22.6							
ATO		712	CA	VAL	1704	33.5		11.40			1.00	35.00	)
ATO		713		VAL	1704	33.6		11.65			1.00	33.25	
OTA		714	CG1		1704	33.6		10.33			1.00	31.04	
ATO		15		VAL	1704	33.8		10.60		766		32.72	
ATO	M 17			VAL	1704	34.8		9.47		727	1.00	26.97	
ATO		17	_	ZAL	1704	32.4		12.52			1.00		
ATO				PRO	1704	31.3		12.15				36.79	
ATON	V 17		-	PRO	1705	32.7		13.735		32	1.00	35.01	
ATON	1 17		_	PRO	1705	34.1		14.333	11.0		1.00	35.61	
ATOM	1 17:		-	RO	1705	31.80		14.685		12	1.00	35.33	
ATOM	1 17:			RO	1705	32.53		16.020				35.59	
ATOM	1 172	_		RO	1705	33.95		15.625		<b>-</b> -		37.23	
ATOM		_		RO		31.38		14.375	9.0			36.33	
ATOM			_	AL	1705	32.12		13.695	8.3			38.44	
ATOM				AL	1706	30.24		14.912				34.93	
ATOM				AL	1706	29.67		14.704	7.30			35.19	
ATOM			G1 V		1706	28.60		15.791	6.98			36.19	
ATOM	172	_	G2 V		1706	28.01		15.586	5.58	_		36.19	
ATOM	173	_			1706	27.49		15.739	8.02			32.74	
ATOM	173	_			1706	30.69		14.632	6.15		00	36.20	
ATOM	173				1706	30.79		13.618	5.46		00	38.16	
ATOM	173				1707	31.479		15.695	6.02		00	34.38	
ATOM	1734				1707	32.500		15.819	4.98		00	33.75	
ATOM	1735		B GI GL		1707	33.181		17.184	5.08		00 :	3.75 35.79	
ATOM	1736				1707	33.567	' ]	14.731	4.98		00 3	55.79 51.97	
ATOM	1737	_	GL GL		1707	34.036		4.311	3.92.		00. 3	2.84	
ATOM	1738				1708	33.964	1	4.280	6.160			9.57	
ATOM	1739				1708	34.987		3.249	6.249		_	1.32	
ATOM	1740				708	35.567		3.204	7.664			6.11	
ATOM	1741				708	36.189		4.508	8.144		00 4	4.10	
ATOM	1742		1 GL		708	37.444		4.923	7.383		00 5		
ATOM	1743		2 GL		708	38.059		4.082	6.681		00 6:	1 47	
ATOM	1744	C	GLU		708	37.830	1	6.115	7.517		00 60		
ATOM	1745	0	GLU		708 700	34.365		1.906	5.889			2.20	
ATOM	1746	N	LEU	_	708 700	35.013		1.041	5.294		00 32	7 70	
ATOM	1747	CA	LEU		709	33.094	1.	1.749	6.245		0 31	4.3	
MOTA	1748	CB	LEU		709	32.378		0.522	5.961			71	
ATOM	1749	CG	LEU	_	709	30.973	10	0.548	6.565	1.0		. 84	
ATOM	1750		LEU	-	709	30.136	9	9.357	6.081		0 28	20	
ATOM	1751		LEU		709	30.662		.059	6.679		0 27		
ATOM	1752	C	LEU		709	28.705		.556	6.437		0 29		
ATOM	1753	0	LEU		09	32.306	10	.317	4.454	1.0	0 30	· / I	
ATOM	1754	N			09	32.489	9	.202	3.970	1.0	0 31	70	
ATOM	1755	CA	PHE		10	32.043	11	.399	3.727	1 0	0 30	. / 9	
ATOM	1756	CB	PHE		10	31.945	11	.366	2.279	1 0	0 32	. 23	
ATOM	1757		PHE		10	31.680	12	.768	1.737	1 00	34.		
ATOM	1758	CG	PHE	17		30.310		.261	2.020		37.		
ATOM	1759		PHE	17		29.337			2.495	1 00	) 43.	43	
ATOM	1760		PHE	17		29.984			1.838	1 00	43.	4.3	
	1761		PHE	17		28.054			2.787	1 00	42.	0/	
	1762		PHE	17:		28.698			2.130	1 00	46.	20	•
-	02	CZ	PHE	17:	Γ0	27.733			2.605		46.		
•										00	-20.	マン	

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ATOM	1763	С	PHE	1710	33.196	10.802	1.667	1.00 34.25
ATOM	1764	0	PHE	1710	33.133	9.948	0.785	1.00 36.09
MOTA	1765	N	LYS	1711	34.324	11.249	2.209	1.00 34.37
MOTA	1766	CA	LYS	1711	35.664	10.840	1.789	1.00 34.11
MOTA	1767	CB	LYS	1711	36.672	11.768	2.476	1.00 37.74
ATOM	1768	CG	LYS	1711	38.114	11.567	2.119	1.00 43.59
MOTA	1769	CD	LYS	1711	38.978	12.573	2.857	1.00 46.97
ATOM	1770	CE	LYS	1711	40.386	12.575	2.304	1.00 51.53
MOTA	1771	NZ	LYS	1711	41.074	11.291	2.603	1.00 58.84
MOTA	1772	С	LYS	1711	35.948	9.354	2.103	1.00 33.25
MOTA	1773	0	LYS	1711	36.512	8.641	1.274	1.00 32.22
MOTA	1774	N	LEU	1712	35.537	8.894	3.285	1.00 32.62
MOTA	1775	CA	LEU	1712	35.718	7.496	3.667	1.00 31.41
ATOM	1776	CB	LEU	1712	35.223	7.237	5.106	1.00 29.80
ATOM	1777	CG	LEU	1712	36.020	7.889	6.244	1.00 29.22
MOTA	1778		LEU	1712	35.385	7.643	7.608	1.00 24.09
ATOM	1779	CD2	LEU	1712	37.437	7.356	6.234	1.00 28.36
ATOM	1780	С	LEU	1712	34. <b>9</b> 39	6.638	2.674	1.00 31.88
ATOM	1781	0	LEU	1712	35.452	5.654	2.143	1.00 34.08
ATOM	1782	N	LEU	1713	33.700	7.029	2.413	1.00 32.28
ATOM	1783	CA	LEU	1713	32.850	6.305	1.482	1.00 35.36
MOTA	1784	CB	LEU	1713	31.433	ნ.887	1.485	1.00 38.97
MOTA	1785	CG	LEU	1713	30.629	6.494	2.730	1.00 39.56
MOTA	1786	CD1	LEU	1713	29.308	7.228	2.768	1.00 37.14
ATOM	1787		LEU	1713	30.424	4.988	2.748	1.00 37.73
MOTA	1788	С	LEU	1713	33.430	6.296	0.070	1.00 36.47
ATOM	1789	0	LEU	1713	33.502	5.244	-0.563	1.00 39.32
MOTA	1790	N	LYS	1714	33.855	7.455	-0.413	1.00 35.21
MOTA	1791	CA	LYS	1714	34.437	7.544	-1.743	1.00 34.55
ATOM	1792	CB	LYS	1714 .	34.812	8.984	-2.075	1.00 34.81
MOTA	1793	CG	LYS	1714	33.624	9.903	-2.290	1.00 36.55
MOTA	1794	CD	LYS	1714	32.681	9.372	-3.353	1.00 40.68
ATOM	1795	CE	LYS	1714	31.488	10.310	-3.577	1.00 44.87
ATOM	1796	NZ	LYS	1714	30.611	9.853	-4.701	1.00 50.99
ATOM	1797	С	LYS	1714	35.671	6.649	-1.856	1.00 35.97
ATOM	1798	0	LYS	1714	35.948	6.084	-2.920	1.00 38.11
ATOM	1799	N	GLU	1715	36.385	6.490	-0.749	1.00 33.65
MOTA	1800	CA	GLU	1715	37.582	5.663	-0.729	1.00 34.34
ATOM	1801	CB	GLU	1715	38.574	6.221	0.288	1.00 34.90
MOTA	1802	CG	GLU	1715	39.032	7.613	-0.110	1.00 42.07
ATOM	1803	CD	GLU	1715	39.729	8.405	0.989	1.00 47.94
ATOM	1804		GLU	1715	39.977	7.870	2.098	1.00 45.03
ATOM	1805	OE2		1715	40.026	9.596	0.709	1.00 51.48
ATOM	1806	C	GLU	1715	37.285	4.191	-0.466	1.00 34.76
ATOM	1807	0	GLU	1715	38.205	3.384	-0.411	1.00 37.36
ATOM	1808	N	GLY	1716	36.002	3.848	-0.347	1.00 32.00
ATOM	1809	CA	GLY	1716	35.604	2.474	-0.122	1.00 30.49
ATOM	1810	C	GLY	1716	35.932	1.937	1.251	1.00 31.32
ATOM	1811	0	GLY	1716	36.134	0.738	1.430	1.00 31.83
ATOM	1812	N	HIS	1717	35.957	2.822	2.233	1.00 31.55
ATOM	1813	CA	HIS	1717	36.265	2.416	3.595	1.00 33.20
MOTA	1814	CB	HIS	1717	36.494	3.661	4.452	1.00 37.67

	OM 1815	CG HIS	1717	36.786 3.360 5.005
	OM 1816	CD2 HIS	1717	37.055 3.360 5.895 1.00 42.42
	OM 1817	ND1 HIS	1717	3.259 6.567 1.00 40 97
	OM 1818	CE1 HIS	1717	3.142 6.825 1.00 45 02
AT		NE2 HIS	1717	2.914 8.004 1.00 44 06
AT	OM 1820	C HIS	1717	2.9/6 7.873 1.00 43 67
ATO		O HIS	1717	1.36/ 4.201 1.00 31 73
ATO		37	1718	33.975 1.816 3.952 1.00 32 12
ATO		C3	1718	35.529 0.582 5.009 1.00 31 00
ATC	OM 1824		1718	34.586 -0.288 5.696 1.00 32 ***
ATC	M 1825	CC		34.531 -1.664 5 024 1 00 5
ATO	M 1826	OD	1718	34.048 -1.651 3 577 1 00 22
ATO		1777	1718	32.579 -1.263 3 495 1 00 00
ATO		00	1718	32.036 -1.320 2 129 1 00 29.60
ATO			718	32.103 -0.324 1 242 1 00 24.72
ATO			718	32.709 0.010
ATO	-050		718	31.463 -0.444
ATO	v 1001		718	35.042 -0.420 - 1.00 14.18
ATON	4		718	36.234 -0.506 7.104 1.00 33.81
ATOM	1 100.		719	34 084 0 370
ATOM	1 200-		719	34 382 0 466 0.005 1.00 33.99
ATOM			719	33 110 0 246
ATOM			719	32 513 1 155
ATOM			719	31 082 1 526
ATOM			719	29 906 0 373
ATOM	2005 (		719	35.033 1 700
ATOM	-010		19	34,900 -2 772
ATOM	-0.1	ASP 17	20	35.776 -7.025 -7.038 1.00 33.67
ATOM			20	36.466 3.020 10.345 1.00 35.49
ATOM		B ASP 17	20	37 585 2 604
ATOM		G ASP 17	20	38 688 7 255
		D1 ASP 17	20	38 507 7 470
ATOM		D2 ASP 17	20	39 740 2 650
ATOM	1847 C	ASP 172	20	35 516 4 006 12.422 1.00 46.76
ATOM	1848 O	ASP 172	20	34.459 -3.503 1.00 34.70
ATOM	1849 N			35 037 12.348 1.00 34.31
ATOM	1850 C	A LYS 172	21	25 110 12:132 1:00 33:39
ATOM	1851 C	3 LYS 172	1	25 (00 2 1.00 32.68
ATOM	1852 CG	F LYS 172	1	34 034 17.690 12.500 1.00 33.55
ATOM	1853 CI			35 336 33.119 1.00 33.62
ATOM	1854 CE	LYS 172	1	33.336 -10.158 12.771 1 00 35
ATOM	1855 NZ			36.002 -10.747 13.931 1.00 38.73
ATOM	1856 C	LYS 172		35.323 -12.190 13.711 1.00 43 86
ATOM	1857 O	LYS 172		36.10/ 14.240 1.00 34.61
ATOM	1858 N	PRO 172		33.057 -5.944 14.905 1.00 37.05
ATOM	1859 CD	PRO 172		32 515
ATOM	1860 CA	PRO 1722		14.066 1.00 34 72
ATOM	1861 CB	PRO 1722		33.611 -5.926 16.222 1.00 37 94
ATOM	1862 CG	PRO 1722		32.095 -6.017 16.360 1.00 37 10
ATOM	1863 C			31.607 -5.448 15.073 1 00 36 05
ATOM	1864 0			34.266 -7.109 16.950 7.00 38.85
ATOM	1865 N			34.340 -8.218 16.406 1.00 38 92
ATOM	1866 CA	SER 1723 SER 1723		34.783 -6.884 18.150 1.00 42 36
		1/23		35.359 -7.995 18.890 1.00 45.70
				2.00 43.70

ATOM	1867	CB	SER	1723	36.170	-7.511	20.093	1.00	47.50
ATOM	1868	OG	SER	1723	35.341	-6.964	21.100	1.00	55.28
ATOM	1869	С	SER	1723	34.136	-8.784	19.346	1.00	46.70
ATOM	1870	0	SER	1723	33.037	-8.224	19.477	1.00	47.27
ATOM	1871	N	ASN	1724	34.296	-10.081	19.559	1.00	47.84
ATOM	1872	CA	ASN	1724	33.174	-10.900	19.992	1.00	51.26
MOTA	1873	CB	ASN	1724	32.620	-10.361	21.330	1.00	57.15
MOTA	1874	CG	ASN	1724	33.732	-10.088	22.365	1.00	61.53
MOTA	1875	OD1	ASN	1724	34.565	-10.955	22.646	1.00	64.13
MOTA	1876	ND2	ASN	1724	33.763	-8.867	22.912	1.00	61.69
ATOM	1877	C	ASN	1724	32.101	-10.916	18.873	1.00	50.72
ATOM	1878	0	ASN	1724	30.925	-10.617	19.089	1.00	52.63
ATOM	1879	N	CYS	1725	32.564	-11.193	17.663	1.00	48.01
MOTA	1880	CA	CYS	1725	31.719	-11.295	16.478	1.00	45.16
ATOM	1881	CB	CYS	1725	31.603	-9.929	15.788	1.00	44.77
ATOM	1882	SG	CYS	1725	30.605	-9.929	14.272	1.00	40.74
ATOM	1883	C	CYS	1725	32.421	-12.308	15.570	1.00	41.51
ATOM	1884	0	CYS	1725	33.639	-12.236	15.397		42.47
ATOM	1885	N	THR	1726	31.677	-13.289	15.064		37.54
ATOM	1886	CA	THR	1726	32.268	-14.313	14.202		35.03
ATOM	1887	CB	THR	1726	31.308	-15.500	13.993		31.87
ATOM	1888	OG1	THR	1726	30.074	-15.042	13.406		32.84
ATOM	1889	CG2	THR	1726	31.017	-16.160	15.306		29.78
ATOM	1890	C	THR	1726	32.678	-13.770	12.845		34.76
MOTA	1891	0	THR	1726	32.180	-12.729	12.415		38.22
ATOM	1892	N	ASN	1727	33.596	-14.450	12.175		32.47
ATOM	1893	CA	ASN	1727	34.009	-14.024	10.842		34.75
ATOM	1894	СВ	ASN	1727	35.167	-14.872	10.308		39.77
ATOM	1895	CG	ASN	1727	36.464	-14.591	11.026		46.09
MOTA	1896	OD1	ASN	1727		-13.495	10.933		49.54
ATOM	1897	ND2	ASN	1727	36.961	-15.585	11.749		50.04
MOTA	1898	С	ASN	1727	32.825	-14.147	9.905		33.38
ATOM	1899	0	ASN	1727	32.726	-13.405	8.929		34.10
ATOM	1900	N	GLU	1728	31.916	-15.065	10.224	1.00	
MOTA	1901	CA	GLU	1728	30.707	-15.310	9.418		30.41
MOTA	1902	СВ	GLU	1728	30.010	-16.580	9.917		32.27
MOTA	1903	CG	GLU	1728	28.811	-17.034	9.094		31.55
ATOM	1904	CD	GLU	1728	28.251	-18.369	9.577		36.38
MOTA	1905	OE1	GLU	1728	28.415	-18.694	10.777	1.00	
ATOM	1906	OE2	GLU	1728		-19.086	8.758	1.00	
ATOM	1907	С	GLU	1728		-14.119	9.468	1.00	
ATOM	1908	0	GLU	1728		-13.679	8.438	1.00	
ATOM	1909	N	LEU	1729		-13.610	10.672	1.00	
ATOM	1910	CA	LEU	1729		-12.462	10.849	1.00	
MOTA	1911	CB	LEU	1729		-12.343	12.310	1.00	
ATOM	1912	CG	LEU	1729		-13.410	12.721	1.00	
ATOM	1913		LEU	1729		-13.377	14.226	1.00	
ATOM	1914		LEU	1729		-13.377	12.010	1.00	
ATOM	1915	C	LEU	1729		-11.161	10.335	1.00	
ATOM	1916	0	LEU	1729		-10.255	9.914	1.00	
ATOM	1917	N	TYR	1730					
ATOM	1918	CA	TYR			-11.069	10.363	1.00	
71 OF	T 3 T O	CA	IIK	1730	31.281	-9.881	9.844	1.00	26.47



ATOM 1919 CB TYR 1730	20
ATOM 1920 CG TVP 1720	32.742 -9.869 10.298 1 00 24 24
ATOM 1921 CD1 TVP 1730	33.512 -8.670 9.805 1 00 25 61
ATOM 1922 CE1 TVP 1730	33.029 -7.373 10.016 1.00 35 50
ATOM 1923 CD2 TYR 1730	33.691 -6.264 9.496 1.00 33.70
ATOM 1924 CE2 TYR 1730	34.688 -8.826 9.067 1.00 24.40
ATOM 1925 CZ TVP 1730	35.361 -7.719 8.537 1.00 22 61
ATOM 1926 OH TYR 1730	34.856 -6.445 8.748 1 00 24 47
1927 C TYR 1730	35.4/6 -5.354 8.176 1.00 24.37
1928 O TYR 1730	31.186 -9.902 8.301 1 00 36 35
1929 N MET 1731	7 651 1 00
1930 CA MET 1731	31.347 -11.084 7 727 2 23.00
ATOM 1931 CB MET 1731	
ATOM 1932 CG MET 1731	31.4/5 -12.740 5 960
A10M 1933 SD MET 1731	31.076 -13.157 4 577
ATOM 1934 CE MET 1731	44.031 A 216 7 8
1935 C MET 1731	***************************************
1936 O MET 1731	40.019 5 040 5
ATOM 1937 N MET 1732	28 045 - 4.791 1.00 30 94
CA MET 1732	6.633 1 00 20
7 MONE 1732	26 537 10.743 6.328 1.00 26.97
ATOM 1732	7.398 1 00 25
ATOM 10.0	23 990 75 7.156 1.00 26.01
ATOM 1015 CE MET 1732	23 772 23 8.407 1.00 26.97
ATOM 1044	27.387 -9.332 7.798 1.00 21.23
ATOM 1945 5	26.778 -9.663 - 1.00 27.49
ATOM 1946 7	27.982 -0.550 3.361 1.00 29.17
ATOM 1047 1121 1/33	28.001 -7.000 7.239 1.00 27.79
ATOM 1040 -	28.797 -6 505 7.293 1.00 27.41
ATOM 1040	28.153 -6.761 9.830 3.84
ATOM 1950 CE MET 1733	29.300 -6.248 11 127
ATOM 1951 C MET 1733	28.850 -7.423 12.200 1.55
ATOM 1952 O MET 1733	20./11 -6.599 6.035 1.03
ATOM 1953 N APC 1734	28.250 -5.680 5.357 1.00 30.60
1954 CA APC 1734	29.865 -7.194 5.751 1 00 20 50
ATOM 1955 CB APC 1734	30.650 -6.831 4.571 1.00 30.53
ATOM 1956 CG ARG 1734	7.009 4.531 1.00 20 74
ATOM 1957 CD ARG 1734	7,245 5,638 1 00 36 ==
1958 NE ARG 1734	5.702 1 00 26 50
1959 CZ ARG 1734	35 130 - 4.499 1.00 34.72
NM1 ARG 1734	35 937 - 3.360 4.306 1.00 37.67
ATOM 1060 TO ARG 1734	35.663 4.006 5.251 1.00 40.46
ATOM 1062 - ARG 1734	29.855 -7.051
ATOM 1064	29.958 6.352 3.294 1.00 28.03
ATOM 1005 0	29.071 8.122 2.359 1.00 27.22
ATOM 1000 ASP 1735	28.212 0.435 3.260 1.00 27.81
ATOM 1000 TO	27 608 2 2.103 1.00 27.27
Amor: CG ASP 1735	28.638 -10.032 2.216 1.00 28.62
ATOM 1969 ODS	29 745 -10 662 2.075 1.00 30.15
ATOM 1970 C 307	28.354 -12.070 2.503 1.00 31.23
1970 C ASP 1735	27,099
200-	1.971 1.00 24.78
SSSD /FF02:	

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ATOM	1971	0	ASP	1735	26.714	-7.068	0.852	1.00	24.52
ATOM	1972	N	CYS	1736	26.590	-6.908	3.104	1.00	24.10
ATOM	1973	CA	CYS	1736	25.530	-5.871	3.140	1.00	25.20
ATOM	1974	CB	CYS	1736	24.965	-5.679	4.569		23.85
MOTA	1975	SG	CYS	1736	23.898	-7.030	5.143	1.00	
MOTA	1976	C	CYS	1736	26.042	-4.520	2.611	1.00	
ATOM	1977	0	CYS	1736	25.276	-3.718	2.070		
ATOM	1978	N	TRP	1737	27.348	-4.303	2.743		23.53
ATOM	1979	CA	TRP	1737	27.988	-3.072	2.302		21.57
ATOM	1980	СВ	TRP	1737	29.026	-2.631	3.314		18.82
ATOM	1981	CG	TRP	1737	28.485	-2.418	4.686		19.89
ATOM	1982		TRP	1737	29.194	-2.609	5.913		22.39
ATOM	1983	CE2		1737	28.329	-2.213	6.959		21.78
ATOM	1984		TRP	1737	30.478	-3.083	6.238		23.52
ATOM	1985		TRP	1737	27.248	-1.932	5.022		19.40
ATOM	1986	NE1		1737	27.147	-1.805	6.383		21.52
ATOM	1987	CZ2		1737	28.705	-2.270	8.319		21.85
ATOM	1988	CZ3	TRP	1737	30.857	-3.134	7.583		25.30
ATOM	1989	CH2	TRP	1737	29.972	-2.728	8.604		26.17
ATOM	1990	С	TRP	1737	28.673	-3.226	0.956		24.49
ATOM	1991	0	TRP	1737	29.648	-2.519	0.670		25.09
ATOM	1992	N	HIS	1738	28.203	-4.170	0.136		25.12
ATOM	1993	CA	HIS	1738	28.808	-4.341	-1.172		22.90
ATOM	1994	СВ	HIS	1738	28.163	-5.497	-1.928		23.14
ATOM	1995	CG	HIS	1738	29.017	-6.013	-3.051		23.26
ATOM	1996		HIS	1738	29.550	-5.380	-4.129		23.78
ATOM	1997		HIS	1738	29.492	-7.308	-3.104		24.91
ATOM	1998		HIS	1738	30.286	-7.445	-4.156	1.00	
ATOM	1999		HIS	1738	30.341	-6.288	-4.794		26.99
ATOM	2000	С	HIS	1738	28.670	-3.024	-1.958	1.00	
ATOM	2001	0	HIS	1738	27.615	-2.381	-1.933	1.00	
ATOM	2002	N	ALA	1739	29.752	-2.608	-2.607	1.00	
ATOM	2003	CA	ALA	1739	29.762	-1.378	-3.385	1.00	
ATOM	2004	СВ	ALA	1739	31.079	-1.234	-4.076	1.00	
ATOM	2005	С	ALA	1739	28.645	-1.391	-4.416	1.00	
ATOM	2006	0	ALA	1739	27.955	-0.391	-4.606	1.00	
MOTA	2007	N	VAL	1740	28.507	-2.521	-5.102	1.00	
ATOM	2008	CA	VAL	1740	27.481	-2.700	-6.121	1.00	
ATOM	2009	CB	VAL	1740	27.966	-3.698	-7.206	1.00	
ATOM	2010	CG1	VAL	1740	27.013	-3.757	-8.360	1.00	
ATOM	2011		VAL	1740	29.308	-3.260	-7.720	1.00	
ATOM	2012	С	VAL	1740	26.170	-3.209	-5.481	1.00	
ATOM	2013	0	VAL	1740	26.126	-4.347	-4.978	1.00	
MOTA	2014	N	PRO	1741	25.090	-2.397	-5.545	1.00	
ATOM	2015	CD	PRO	1741	25.074	-1.093	-6.237	1.00	
ATOM	2016	CA	PRO	1741	23.763	-2.695	-4.980	1.00	
ATOM	2017	CB	PRO	1741	22.891	-1.554	-5.526	1.00	
ATOM	2018	CG	PRO	1741	23.866	-0.419	-5.647	1.00	
ATOM	2019	c	PRO	1741	23.189	-4.074	-5.343	1.00	
ATOM	2020	Ō	PRO	1741	22.700	-4.788	-4.462	1.00 2	
ATOM	2021	N	SER	1742	23.335	-4.473	-6.615	1.00 2	
ATOM	2022	CA	SER	1742	22.826	-5.754	-7.119	1.00 2	
						~		1.00	,_,

ית	TOM 2023			
			SER 1742	
	FOM 2024		SER 1742	24 324 5 200
	TOM 2025	С	SER 1742	23 524 5 001
	OM 2026	0	SER 1742	22 202 - 3.343 1.00 23.09
	OM 2027	N (	GLN 1743	24 710 -6.603 1.00 21.90
AT		CA (	3LN 1743	
AT		CB (	GLN 1743	-7.895 -5.416 1.00 23 26
AT	-,00	CG G	SLN 1743	20.333 -7.754 -5.702 1.00 24 32
ATO	OM 2031		LN 1743	27.233 -7.828 -7.170 1.00 23 04
ATO		OE1 G		26.684 -9.076 -7 R10 1 00 0
ATO	DM 2033		LN 1743	27.176 -10.178 -7.584 1.00 21.07
ATC		_		<sup>25.647</sup> -8.907 -8.625 1.00 20 5-
ATC	DM 2035	_		25.227 -8.121 -3.927 1 00 22.55
ATC	M 2036	_		<sup>25.744</sup> -9.083 -3.366 1.00.05 a.
ATO				24.458 -7.240 -3.290 1.00 23.36
ATO		_	- · • •	24.155 -7.395 -1.868 1.00 22.69
ATO.			RG 1744	23 635
ATO	M 2011	_		24 627 4 255
ATO	M 22	CD AF		24 013 3 656
ATO		NE AR		24 869 2 563 1.00 19.06
ATON		CZ AR		24 461 1 222
ATON		NH1 AR	- <del>-</del>	23.184 0.070
ATOM		NH2 AR		25 337 0 438 1.00 18.95
ATOM	1 22.0	C AR	-	23 095 0 470
ATOM		) AR		22 363 0 === 1.712 1.00 22.45
ATOM		1 PR	7 1745	23 065 0 175
ATOM		D PRO	1745	24 025 0 20
ATOM		'A PRO	1745	22 057 10 175
ATOM		B PRO	1745	22 532 10 000
		G PRO	1745	23 240 0 777
ATOM	-552 C	PRO	1745	20 726 0 107 1.676 1.00 19.86
ATOM	•	PRO	1745	20 600 -9.485 -0.146 1.00 22.18
ATOM	2054 N	THR	1746	10.646 281 0.128 1.00 23.04
ATOM	2055 C	A THR		10.236 -0.297 1.00 19.31
ATOM	2056 CI	3 THR		17 305 -9.689 -0.085 1.00 19.12
ATOM		31 THR	1746	-7.307 -10.334 -1.045 1.00 19 gc
ATOM	2058 CC	2 THR	1746	-1,2,3 -11,763 -0.886 1 00 00 -
ATOM	2059 C	THR	1746	-7.000 -10.002 -2.479 1.00 22 97
ATOM	2060 O	THR	1746	-7.501 -9.9/5 1.367 7.00 10
ATOM	2061 N	PHE	1747	18.676 -10.711 2.058 1.00 19.93
MOTA	2062 CA		1747	16.884 -9.381 1.855 1.00 21.05
ATOM	2063 CB		1747	16.456 -9.678 3.224 1.00 23 46
ATOM	2064 CG			15.353 -8.720 3.686 1.00 01.5
ATOM		1 PHE	1747	15.872 -7.368 4.082 1.00 24.04
ATOM		2 PHE	1747	16.627 -7.207 5.237 1.00 22.04
ATOM			1747	15 611
ATOM		l PHE	1747	17 124 5 22.97
ATOM		PHE	1747	16 111 4 22
ATOM		PHE	1747	16 862 4 815
ATOM		PHE	1747	15 992 11 122
ATOM	2071 0	PHE	1747	16 189 11 704
ATOM	2072 N	LYS	1748	15 430 11 620
ATOM	2073 CA	LYS	1748	14. 971 13.01
ATOM	2074 CB	LYS	1748	14 344 12 22
				14.344 -13.327 0.782 1.00 26.89
CCCD/FF				

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ATOM	2075	CG	LYS	1748	14.061	-14.793	0.583	1.00	31.07
ATOM	2076	CD	LYS	1748		-15.064	-0.861	1.00	37.82
ATOM	2077	CE	LYS	1748	13.231	-16.493	-1.068	1.00	44.36
MOTA	2078	NZ	LYS	1748	12.027	-16.782	-0.235	1.00	50.16
MOTA	2079	С	LYS	1748	16.160	-13.949	2.393	1.00	27.27
ATOM	2080	0	LYS	1748	16.067	-14.877	3.202	1.00	27.87
MOTA	2081	N	GLN	1749	- 17.288	-13.674	1.730	1.00	25.64
ATOM	2082	CA	GLN	1749	18.507	-14.457	1.903	1.00	24.32
ATOM	2083	CB	GLN	1749	19.608	-13.938	0.983	1.00	28.87
MOTA	2084	CG	GLN	1749	19.343	-14.049	-0.496	1.00	36.24
ATOM	2085	CD	GLN	1749	20.437	-13.374	-1.318	1.00	41.30
MOTA	2086	OE1	GLN	1749	20.173	-12.422	-2.044	1.00	38.35
MOTA	2087	NE2	GLN	1749	21.683	-13.861	-1.190	1.00	45.38
MOTA	2088	C	GLN	1749	19.002	-14.310	3.346	1.00	22.89
ATOM	2089	0	GLN	1749	19.302	-15.305	4.008	1.00	22.55
ATOM	2090	N	LEU	1750	19.114	-13.064	3.813	1.00	20.89
ATOM	2091	CA	LEU	1750	19.570	-12.776	5.167	1.00	21.44
ATOM	2092	CB	LEU	1750	19.471	-11.282	5.462	1.00	19.53
MOTA	2093	CG	LEU	1750	20.432	-10.400	4.663	1.00	19.14
ATOM	2094	CD1	LEU	1750	20.069	-8.919	4.816	1.00	14.53
ATOM	2095	CD2	LEU	1750	21.863	-10.685	5.106	1.00	16.18
MOTA	2096	С	LEU	1750	18.776	-13.538	6.208	1.00	22.98
MOTA	2097	0	LEU	1750	19.335	-14.057	7.183	1.00	23.12
MOTA	2098	N	VAL	1751	17.465	-13.586	6.020	1.00	23.48
ATOM	2099	CA	VAL	1751	16.610	-14.292	6.945		23.21
MOTA	2100	CB	VAL	1751	15.132	-14.075	6.590	1.00	20.94
ATOM	2101		VAL	1751	14.268	-15.008	7.375	1.00	21.67
MOTA	2102		VAL	1751	14.730	-12.649	6.929		20.32
ATOM	2103	С	LAV	1751	16.974	-15.774	6.990	1.00	26.13
ATOM	2104	0	VAL	1751		-16.379	8.058		26.35
ATOM	2105	N	GLU	1752	17.260	-16.348	5.831	1.00	30.05
ATOM	2106	CA	GLU	1752		-17.747	5.778		32.54
ATOM	2107	CB	GLU	1752		-18.221	4.338		38.54
ATOM	2108	CG	GLU	1752		-18.226	3.673		50.06
MOTA	2109	CD	GLU	1752		-18.759	2.247		56.55
MOTA	2110		GLU	1752		-18.480	1.507		61.63
MOTA	2111	OE2	GLU	1752		-19.466	1.875		59.57
MOTA	2112	C	GLU	1752		-17.965	6.486		31.62
ATOM	2113	0	GLU	1752		-18.858	7.322		29.63
ATOM	2114	N	ASP	1753		-17.103	6.193	1.00	
ATOM	2115	CA	ASP	1753		-17.211	6.807	1.00	
ATOM	2116	CB	ASP	1753		-16.181	6.203	1.00	
ATOM	2117	CG	ASP	1753		-16.390	4.710	1.00	
ATOM	2118	OD1		1753		-17.549	4.248	1.00	
ATOM	2119	OD2		1753		-15.396	3.992	1.00	
ATOM	2120	C	ASP	1753		-17.058	8.314	1.00	
ATOM	2121	0	ASP	1753		-17.933	9.059	1.00	
ATOM	2122	N	LEU	1754		-15.984	8.764	1.00	
ATOM	2123	CA	LEU	1754		-15.731	10.199	1.00	
ATOM	2124	CB	LEU	1754		-14.372	10.457	1.00	
ATOM	2125	CG	LEU	1754		-13.269	10.154	1.00	
MOTA	2126	CD1	LEO	1754	20.074	-11.886	9.995	1.00	14.83

AT		CD2 LEU	1754	21 22-
ATO	0	C LEU		21.831 -13.308 11.240 1.00 16.39
ATO	,	O LEU	-	20,020 -16.861 10.896 1.00 29.18
ATC		N ASP		20.030 -17.262 11.986 1 00 20 55
ATC		CA ASP	1755	17 000 17.421 10.238 1.00 31.65
ATO		CB ASP	1755	16 733
ATO		CG ASP	1755	15.723 -18.900 9.928 1.00 34.57
ATO		OD1 ASP	1755	15.676 -19.997 10.533 1.00 38.29
ATO		OD2 ASP	1755	13.410 -19.844 11.677 1.00 45 55
ATO		C ASP	1755	10.005 -21.031 9.878 1.00 43.09
ATO		O ASP	1755	19.665 11.034 1.00 33.50
ATO		N ARG	1756	10.730 120.428 12.025 1.00 34.39
ATON		CA ARG	1756	20.700 -19.90/ 10.107 1.00 35.51
ATOM		CB ARG	1756	21 417 22 1004 10.169 1.00 35.33
ATOM	_	CG ARG	1756	32 522 8.825 1.00 38.41
ATOM		CD ARG	1756	22.181 8.759 1.00 40.99
ATOM		NE ARG	1756	7 376 1 00 44
ATOM	- <del>-</del>	CZ ARG	1756	24 705 -20.917 6.916 1.00 49.55
ATOM	·· <del>-</del>	NH1 ARG	1756	25.555 -20.338 7.349 1.00 53.56
ATOM	•	NH2 ARG	1756	25.350 120.937 8.266 1.00 53.25
ATOM		C ARG	1756	21 710 -19.163 6.853 1.00 55.72
ATOM	0	O ARG	1756	22 000 21 11.275 1.00 35.01
ATOM		N ILE	1757	22 244 10 525
ATOM		CA ILE	1757	23 242 10 15
ATOM		CB ILE	1757	23 847 17 773
ATOM	<b>.</b> .		1757	24 916 17 40-
ATOM		G1 ILE	1757	24 491 12 7-7
ATOM ATOM		D1 ILE	L757	24 812 16 33.64
ATOM	2155		1757	22 673 10 105
ATOM	2156 C		.757	23 293 30 75
MOTA	2157 N		758	21 499 19 600
ATOM	<b>-</b>		758	20 254 30 505
ATOM			758	19 378 -10 70.
ATOM		G1 VAL 1	758	18 715 10 102
ATOM			758	19 309 16 675
ATOM	2		758	20 905 10 055
ATOM			758	21 402 20 43.92
ATOM	2164 N 2165 C		759	20 370 30 05
ATOM	2166 CE		759	20.325 -22.354 15.528 1.00 43.96
ATOM	2167 C		759	19.653 -23.197 14 460 1 00 43.47
ATOM	2168 0		759	21.69322.953 15.890 1.00 44.25
ATOM	2169 N		759	21.780 -23.872 16.697 1.00 45.04
ATOM	2170 CA		60	22.750 -22.465 15.255 1.00 45.07
ATOM	2171 CB		60	24.095 -22.949 15.514 1.00 45.07
ATOM	2172 CG		60	24.899 -22.900 14.225 1.00 48.72
ATOM			60	24.279 -23.645 13.053 1.00 51.00
ATOM		1 LEU 17		25.016 -23.279 11.778 1.00 55 1.98
ATOM	2175 C	2 LEU 17		24.327 -25.136 13.313 1.00 53.19
ATOM	2176 0	LEU 17		24.811 -22.118 16.578 1 00 47 55
	2177 N	LEU 17		25.935 -22.432 16.986 1.00 44.59
	2178 CA	THR 170		24.181 -21.031 17.004 1.00 49.33
	- · • CM	THR 176	) T	24.791 -20.166 17.987 1.00 50.15
				2.00 30.15



ATOM	2179	СВ	THR	1761	24.309	-18.707	17.811	1.00 49.78
MOTA	2180	OG1	THR	1761	24.650	-18.262	16.489	1.00 49.83
ATOM	2181	CG2	THR	1761	24.997	-17.793	18.809	1.00 49.37
ATOM	2182	C	THR	1761	24.643	-20.655	19.426	1.00 51.84
ATOM	2183	0	THR	1761	23.565	-21.064	19.866	1.00 51.38
ATOM	2184	N	SER	1762	25.761	-20.622	20.143	1.00 53.45
ATOM	2185	CA	SER	1762	25.835	-21.042	21.533	1.00 53.79
ATOM	2186	CB	SER	1762	27.301	-21.039	21.969	1.00 58.33
MOTA	2187	OG	SER	1762	27.502	-21.759	23.173	1.00 63.27
MOTA	2188	C	SER	1762	25.033	-20.081	22.403	1.00 50.43
MOTA	2189	0	SER	1762	25.193	-18.856	22.301	1.00 48.42
MOTA	2190	N	ALA	461	79.680	25.808	14.502	1.00 57.40
MOTA	2191	CA	ALA	461	79.609	24.651	13.610	1.00 53.47
ATOM	2192	CB	ALA	461	78.307	23.875	13.860	1.00 54.34
ATOM	2193	С	ALA	461	79.707	25.105	12.151	1.00 49.53
MOTA	2194	0	ALA	461	79.739	24.289	11.243	1.00 48.04
MOTA	2195	N	ALA	462	79.814	26.417	11.957	1.00 46.57
MOTA	2196	CA	ALA	462	79.919	27.014	10.634	1.00 43.66
MOTA	2197	CB	ALA	462	80.034	28.532	10.750	1.00 43.87
MOTA	2198	C	ALA	462	81.074	26.461	9.806	1.00 39.75
MOTA	2199	0	ALA	462	80.869	26.036	8.673	1.00 36.18
ATOM	2200	N	TYR	463	82.279	26.449	10.383	1.00 37.82
ATOM	2201	CA	TYR	463	83.477	25.959	9.686	1.00 36.88
ATOM	2202	СВ	TYR	463	84.615	26.968	9.7€5	1.00 39.12
ATOM	2203	CG	TYR	463	84.372	28.176	8.894	1.00 45.68
ATOM	2204	CD1	TYR	463	84.071	29.422	9.456	1.00 46.07
ATOM	2205	CEl	TYR	463	83.783	30.518	8.652	1.00 48.07
ATOM	2206	CD2	TYR	463	84.384	28.064	7.501	1.00 47.80
MOTA	2207	CE2	TYR	463	84.096	29.154	6.690	1.00 45.55
ATOM	2208	CZ	TYR	463	83.796	30.372	7.271	1.00 47.44
ATOM	2209	ОН	TYR	463	83.491	31.442	6.476	1.00 49.77
ATOM	2210	C	TYR	463	83.988	24.579	10.024	1.00 34.97
ATOM	2211	0	TYR	463	84.605	23.947	9.175	1.00 35.48
ATOM	2212	N	GLU	464	83.761	24.109	11.244	1.00 34.33
ATOM	2213	CA	GLU	464	84.224	22.769	11.630	1.00 36.96
MOTA	2214	CB	GLU	464	. 85.725	22.790	11.901	1.00 41.01
ATOM	2215	CG	GLU	464	86.123	23.764	12.991	1.00 45.91
MOTA	2216	CD	GLU	464	87.619	24.009	13.075	1.00 53.97
ATOM	2217		GLU	464	88.013	24.922	13.835	1.00 58.84
ATOM	2218	OE2	GLU	464	88.400	23.311	12.383	1.00 56.78
ATOM	2219	C	GLU	464	83.517	22.294	12.875	1.00 34.98
ATOM	2220	0	GLU	464	83.252	23.106	13.763	1.00 35.30
ATOM	2221	N	LEU	465	83.193	21.003	12.939	1.00 33.52
MOTA	2222	CA	LEU	465	82.527	20.449	14.121	1.00 35.65
MOTA	2223	CB	LEU	465	81.520	19.348	13.762	1.00 32.97
MOTA	2224	CG	LEU	465	80.488	19.538	12.651	1.00 33.16
MOTA	2225	CD1		465	79.356	18.544	12.911	1.00 27.30
ATOM	2226	CD2	LEU	465	79.983	20.981	12.596	1.00 29.96
MOTA	2227	C	LEU	465	83.572	19.862	15.058	1.00 38.14
MOTA	2228	0	LEU	465	84.707	19.573	14.642	1.00 35.58
MOTA	2229	N	PRO	466	83.215	19.684	16.338	1.00 39.91
ATOM	2230	CD	PRO	466	81.929	20.073	16.942	1.00 42.38

ATO			A PRO	466	84.11	8 19.12	6 17 24	
ATO		_	B PRO	466	83.26			
ATO			G PRO	466	82.32			
ATO		34 C	PRO	466	84.47			
ATON		35 O	PRO		83.68	_		
ATOM		36 N	GLU		85.664			
ATOM		37 C	A GLU		86.106			
ATOM		18 CI	B GLU		87.569			
ATOM		9 C	GLU	467	88.000			,23
ATOM		0 CI	GLU	467	89.372			1.00 59.47
ATOM			E1 GLU	467	90.123			1.00 63.95
ATOM			E2 GLU	467	89.697			1.00 62.08
MOTA		3 C	GLU	467	85.892			1.00 66.76
ATOM	224	4 0	GLU	467	85.988	_		1.00 44.81
MOTA	224	5 N	ASP	468				1.00 45.53
ATOM	224	6 CA		468	85.572	_		1.00 43.85
ATOM	224	7 CB		468	85.357		18.903	1.00 43.44
ATOM	2248	G CG		468	83.872	12.582	19.247	1.00 43.33
ATOM	2249		1 ASP	468	83.611	11.659	20.420	1.00 44.52
ATOM	2250		2 ASP	468	82.452	11.613	20.888	1.00 48.19
ATOM	2251		ASP	468	84.557	10.985	20.877	1.00 42.43
ATOM	2252	0	ASP	468	85.887 85.158	11.411	18.299	1.00 42.37
ATOM	2253	N	PRO	469		10.644	17.669	1.00 43.22
ATOM	2254	CD	PRO	469	87.194	11.182	18.433	1.00 40.72
ATOM	2255	CA	PRO	469	88.167	12.102	19.045	1.00 40.30
ATOM	2256	CB	PRO	469	87.861	9.992	17.909	1.00 39.00
ATOM	2257	CG	PRO	469	89.228	10.078	18.570	1.00 39.03
ATOM	2258	С	PRO	469	89.484	11.564	18.551	1.00 38.11
ATOM	2259	0	PRO	469	87.173	8.663	18.229	1.00 39.37
ATOM	2260	N	ARG	470	87.235	7.718	17.442	1.00 39.27
ATOM	2261	CA	ARG	470	86.497 85.814	8.596	19.371	1.00 39.93
ATOM	2262	CB	ARG	470	85.030	7.374		1.00 42.32
ATOM	2263	CG	ARG	470	85.766	7.614		1.00 46.12
ATOM	2264	CD	ARG	470	84.839	8.370	22.149	1.00 50.76
ATOM	2265	NE	ARG	470	83.649	8.592		1.00 52.76
ATOM	2266	CZ	ARG	470	82.770	9.362		1.00 54.47
ATOM	2267	NH1		470	82.770	9.823		1.00 59.36
MOTA	2268	NH2		470	81.712	9.597		1.00 61.19
ATOM	2269	С	ARG	470	84.814	10.508		L.00 62.88
ATOM	2270	0	ARG	470	84.670	6.896		L.00 42.79
ATOM	2271	N	TRP	471	84.139	5.700		1.00 45.63
ATOM	2272	CA	TRP	471	83.100	7.844		00 41.98
ATOM	2273		TRP	471	81.844			00 38.34
ATOM	2274		TRP	471	81.195			.00 35.68
ATOM	2275	CD2		471	80.388		<b>18</b> .670 1	.00 37.42
ATOM	2276	CE2		471	79.961		18.772 1	.00 37.19
MOTA	2277	CE3		471			20.112 1	.00 36.99
ATOM	2278	CD1		471	79.987		17.855 1	.00 37.80
MOTA	2279	NE1		471	81.223		19.923 1	.00 33.34
		CZ2		471	80.486		20.794 1	.00 34.46
ATOM		CZ3		471	79.150		20.559 1	.00 38.31
		CH2		471	79.180		18.303 1	.00 36.97
		•			78.772	4.506		.00 36.14



MOTA	2283	C	TRP	471	83.409	7.830	15.641	1.00 38.26
MOTA	2284	0	TRP	471	82.655	7.430	14.749	1.00 38.72
MOTA	2285	N	GLU	472	84.478	8.569	15.397	1.00 37.71
ATOM	2286	CA	GLU	472	84.839	8.951	14.041	1.00 38.43
ATOM	2287	CB	GLU	472	86.014	9.924	14.087	1.00 37.56
MOTA	2288	CG	GLU	472	86.146	10.835	12.871	1.00 37.26
ATOM	2289	CD	GLU	472	84.930	11.728	12.625	1.00 39.02
MOTA	2290	OE1	GLU	472	84.361	12.301	13.571	1.00 40.26
ATOM	2291	OE2	GLU	472	84.568	11.879	11.445	1.00 39.35
MOTA	2292	С	GLU	472	85.135	7.806	13.069	1.00 38.32
ATOM	2293	0	GLU	472	85.872	6.875	13.386	1.00 38.11
ATOM	2294	N	LEU	473	84.535	7.884	11.883	1.00 38.44
ATOM	2295	CA	LEU	473	84.775	6.893	10.848	1.00 37.19
ATOM	2296	CB	LEU	473	83.505	6.112	10.511	1.00 35.38
ATOM	2297	CG	LEU	473	83.805	4.910	9.599	1.00 36.49
ATOM	2298		LEU	473	84.365	3.748	10.406	1.00 34.47
MOTA	2299	CD2	LEU	473	82.556	4.452	8.859	1.00 37.55
ATOM	2300	С	LEU	473	85.283	7.623	9.601	1.00 38.21
ATOM	2301	0	LEU	473	84.696	8.631	9.187	1.00 38.52
ATOM	2302	N	PRO	474	86.412	7.156	9.025	1.00 37.74
ATOM	2303	CD	PRO	474	87.292	6.107	9.568	1.00 36.38
ATOM	2304	CA	PRO	474	87.010	7.753	7.824	1.00 36.91
ATOM	2305	CB	PRO	474	88.233	6.865	7.587	1.00 34.65
ATOM	2306	CG	PRO	474	88.620	6.477	8.967	1.00 32.99
ATOM	2307	С	PRO	474	86.036	7.663	6.660	1.00 38.15
ATOM	2308	0	PRO	474	85.536	6.578	6.362	1.00 38.24
ATOM	2309	N	ARG	475	85.793	8.784	5.981	1.00 38.90
MOTA	2310	CA	ARG	475	84.846	8.802	4.863	1.00 41.23
ATOM	2311	CB	ARG	475	84.743	10.206	4.258	1.00 38.36
ATOM	2312	CG	ARG	475	84.311	11.271	5.267	1.00 35.30
ATOM	2313	CD	ARG	475	84.282	12.691	4.679	1.00 35.23
ATOM	2314	NE	ARG	475	83.850	13.658	5.679	1.00 27.27
ATOM	2315	CZ	ARG	475	82.585	13.859	6.011	1.00 25.77
ATOM	2316		ARG	475	81.630	13.181	5.402	1.00 25.09
ATOM ATOM	2317		ARG	475	82.286	14.639	7.047	1.00 25.24
ATOM	2318 2319	C O	ARG ARG	475 475	85.101	7.745	3.791	1.00 42.43
MOTA	2319	N	ASP	476	84.160 86.359	7.212 7.381	3.204	1.00 44.06
MOTA	2321	CA	ASP	476	86.690	6.384	3.594	1.00 44.69
ATOM	2322	CB	ASP	476	88.197	6.371	2.583 2.319	1.00 48.37 1.00 52.12
ATOM	2323	CG	ASP	476	88.988	5.925		1.00 56.56
ATOM	2323		ASP	476	89.299	4.718	3.521 3.613	
ATOM	2325		ASP	476	89.294	6.779	4.376	1.00 59.72 1.00 61.19
ATOM	2326	C	ASP	476	86.210	4.988	2.973	1.00 49.50
ATOM	2327	0	ASP	476	86.204	4.074	2.145	1.00 49.30
ATOM	2328	N	ARG	477	85.852	4.814	4.241	1.00 48.26
ATOM	2329	CA	ARG	477	85.357	3.525	4.732	1.00 48.26
ATOM	2330	CB	ARG	477	85.909	3.252	6.126	1.00 47.16
ATOM	2331	CG	ARG	477	87.325	2.723	6.088	1.00 49.76
ATOM	2332	CD	ARG	477	88.043	2.723	7.406	1.00 53.26
ATOM	2333	NE	ARG	477	87.394	2.213	8.517	1.00 58.02
ATOM	2334	CZ	ARG	477	87.810		9.776	
	~JJ4	-2	and.	7//	87.810	2.297	3.110	1.00 63.35



AT	гом ;	2335	AT7 1 2							
		2336	NH1		477	88.8	75 3.0	32 10.0	21 2 22	
		2336	NH2		477	87.1	39 1.6			64.92
AT			_	<b>ARG</b>	477	83.8	22 3.4	_		66.00
АТ		2338		ARG	477	83.2				45.38
AT		339		LEU	478	83.1			_	43.67
ATO		340		ŒU	478	81.72		_		12.09
		341		ΈU	478	81.19				37.74
AT(		342		EU	478	79.67			-	2.19
ATO		343	CD1 L	EU	478	79.14				0.21
ATC		344	CD2 L	ÉU	478	79.31			3 1.00 2	2.82
ATC		345			478					4.82
ATC		346	O L		478	81.32	_		1.00 3	8.75
ATO		347			179	81.81			1.00 4	0.60
ATO	M 23	348			179	80.47			1.00 3	8 7g
ATO:	M 23	49	CB V		179	80.02		8 0.544		7.97
ATO	M 23		CG1 V			80.35		5 -0.360	1.00 36	, , , , , , , , , , , , , , , , , , ,
ATO			CG2 VA	_	79	79.83		0 -1.759		
ATO			C VA	_	79	81.868		6 -0.405	- 0.	3.55
ATON	4 23			_	79	78.523	4.298			3.76
ATON	·-	_ '	•••		79	77.750	3.383		1.00 37	
ATOM					80	78.127	5.542			7.70
ATOM					80	<sup>7</sup> 6.723	5.942			.32
ATOM			B LE G LE		80	76.630	7.458			.41
ATOM					30	77.287	8.226		1.00 38	.29
ATOM			D1 LE		30	77.098	9.730		1.00 37	.99
ATOM			D2 LET		30	76.666	7.785		1.00 34	.00
ATOM						75.893	5.287		1.00 32	. 79
ATOM		_			0	76.315	5.205		1.00 38	. 24
ATOM					1	74.672	4.896	-1.903	1.00 39.	.11
ATOM	236		A GLY	48	1	73.811	4.223	-0.394	1.00 36.	70
ATOM	236		GLY	48	1	72.417	4.782	-1.357	1.00 36.	53
	236	_	GLY	48	1	72.159	5.961	-1.524	1.00 37.	61
ATOM	236		LYS	48	2	71.484		-1.277	1.00 40.	02
ATOM	236		LYS	48	2	70.099	3.913	-1.911	1.00 37.	52
ATOM	2368		LYS	48	2	69.243	4.313	-2.153	1.00 39.	89
ATOM	2369		LYS	482	2	69.447	3.104	-2.551	1.00 42.	44
ATOM	2370		LYS	482		69.538	5.028	-0.984	1.00 41.	25
ATOM	2371		PRO	483		68.779	4.589	0.163	1.00 42.2	22
ATOM	2372		PRO	483		68.643	6.156	-1.263	1.00 41.	71
ATOM	2373		PRO	483			6.876	-2.537	1.00 41.0	)1
ATOM	2374	CB	PRO	483		68.118	6.889	-0.193	1.00 42.7	
ATOM	2375		PRO	483		67.606	8.146	-0.906	1.00 41.2	
ATOM	2376	С	PRO	483		67.425	7.713	-2.290	1.00 40.1	6
ATOM	2377	0	PRO	483		66.999	6.061	0.429	1.00 44.6	9
ATOM	2378	N	LEU			66.306	5.314		1.00 45.2	<i>-</i>
ATOM	2379	CA	LEU	484		66.883	6.163		.00 45.3	4
MOTA	2380	CB	LEU	484		65.872	5.450		00 47.3	
ATOM	2381	CG		484		66.494	4.793		00 47.3	4
ATOM	2382		LEU LEU	484		67.517	3.668		00 30 -	J n
ATOM	2383	CDJ	TEU	484		68.208	3.337		.00 39.50	<b>.</b>
ATOM	2384		LEU	484		66.861	2.419		.00 33.64	<u>.</u>
ATOM	2385	C	LEU	484		64.733	6.391		.00 33.44	Į.
ATOM		0	LEU	484		63.611	5.941		.00 52.14	ł
	2386	N	GLY	485		65.013	7.697	3.142 1	.00 53.64	t
							,	3.025 1	.00 55.25	II.

MOTA	2387	CA	GLY	485	63.982	8.653	3.427	1.00 58.76
MOTA	2388	С	GLY	485	64.441	10.104	3.503	1.00 60.58
ATOM	2389	0	GLY	485	65.640	10.376	3.600	1.00 61.49
ATOM	2390	N	ALA	486	63.490	11.032	3.489	1.00 61.46
ATOM	2391	CA	ALA	486	63.791	12.458	3.545	1.00 63.24
MOTA	2392	CB	ALA	486	63.847	13.035	2.126	1.00 64.42
ATOM	2393	C	ALA	486	62.730	13.179	4.355	1.00 63.86
ATOM	2394	0	ALA	486	61.655	12.633	4.599	1.00 65.24
MOTA	2395	N	GLY	487	63.022	14.404	4.768	1.00 63.89
MOTA	2396	CA	GLY	487	62.054	15.158	5.538	1.00 64.30
ATOM	2397	С	GLY	487	62.431	16.617	5.623	1.00 65.34
MOTA	2398	0	GLY	487	63.071	17.154	4.718	1.00 65.98
MOTA	2399	N	ALA	488	62.023	17.259	6.711	1.00 66.16
ATOM	2400	CA	ALA	488	62.317	18.666	6.934	1.00 66.71
ATOM	2401	CB	ALA	488	61.647	19.132	8.219	1.00 70.05
MOTA	2402	С	ALA	488	63.828	18.844	7.027	1.00 66.55
ATOM	2403	0	ALA	488	64.432	18.547	8.063	1.00 65.59
ATOM	2404	N	PHE	489	64.430	19.228	5.904	1.00 65.54
MOTA	2405	CA	PHE	489	65.875	19.457	5.807	1.00 65.40
ATOM	2406	CB	PHE	489	66.244	20.775	6.498	1.00 67.06
ATOM	2407	С	PHE	489	66.773	18.296	6.311	1.00 64.01
ATOM	2408	0	PHE	489	67.942	18.502	6.651	1.00 62.51
MOTA	2409	N	GLY	490	66.234	17.075	6.288	1.00 61.41
MOTA	2410	CA	GLY	490	66.974	15.901	6.724	1.00 55.89
MOTA	2411	С	GLY	490	66.858	14.821	5.667	1.00 53.58
ATOM	2412	0	GLY	490	65. <b>8</b> 25	14.703	5.000	1.00 54.22
ATOM	2413	N	GLN	491	67.899	14.006	5.543	1.00 51.23
ATOM	2414	CA	GLN	491	67.966	12.934	4.556	1.00 47.90
MOTA	2415	CB	GLN	491	68.823	13.445	3.387	1.00 50.09
ATOM	2416	CG	GLN	491	. 68.979	12.529	2.183	1.00 56.77
ATOM	2417	CD	GLN	491	69.945	13.115	1.161	1.00 60.83
ATOM	2418	OEl	GLN	491	70.283	14.292	1.218	1.00 65.11
ATOM	2419	NE2	GLN	491	70.411	12.284	0.232	1.00 63.81
MOTA	2420	C	GLN	491	68.597	11.673	5.190	1.00 45.27
ATOM	2421	0	GLN	491	69.507	11.758	6.014	1.00 45.41
ATOM	2422	N	VAL	492	68.112	10.503	4.805	1.00 41.69
MOTA	2423	CA	VAL	492	68.624	9.245	5.325	1.00 39.95
MOTA	2424	CB	VAL	492	67.583	8.528	6.230	1.00 41.77
ATOM	2425	CG1	VAL	492	68.117	7.168	6.701	1.00 39.86
MOTA	2426	CG2	VAL	492	67.226	9.399	7.421	1.00 42.87
ATOM	2427	С	VAL	492	68.911	8.348	4.126	1.00 38.86
MOTA	2428	0	VAL	492	68.025	8.114	3.301	1.00 37.55
ATOM	2429	N	VAL	493	70.141	7.862	4.010	1.00 36.01
MOTA	2430	CA	VAL	493	70.481	6.994	2.895	1.00 37.55
ATOM	2431	CB	VAL	493	71.471	7674	1.889	1.00 38.65
MOTA	2432	CG1	VAL	493	71.128	9.137	1.709	1.00 37.08
ATOM	2433	CG2	VAL	493	72.929	7.498	2.318	1.00 39.03
MOTA	2434	С	VAL	493	71.071	5.678	3.371	1.00 38.61
MOTA	2435	0	VAL	493	71.645	5.599	4.456	1.00 39.75
MOTA	2436	N	LEU	494	70.899	4.637	2.572	1.00 39.68
MOTA	2437	CA	LEU	494	71.460	3.345	2.910	1.00 40.98
MOTA	2438	CB	LEU	494	70.748	2.241	2.123	1.00 42.14



ATC		139	CG L	EU 494	71.29	50 00	00	_
ATC		40	CD1 L		14.4.	-		10.33
ATO		41	CD2 L	EU 494	70.43			
ATO		42		EU 494	72.91			
ATO	M 24	43	O L	EU 494			_	1.00 40.66
ATO	M 24	44	N AI		73.24			
ATO		45	CA AI		73.79	_		1.00 39.74
ATO	M 24	46	CB AL		75.20			
ATO	M 24	47	C AL		75.85	_		1.00 42.91
ATON	1 24	48 (	O AL		75.88			1.00 43.34
ATON			N GL		75.27	-		1.00 43.81
ATON			CA GL		77.14			1.00 44.40
ATOM			CB GL		77.91		4 3.297	1.00 45.12
ATOM			CG GT		78.282		2 2.106	1.00 48.62
ATOM			D GL		77.062		6 1.346	1.00 56.98
ATOM		_	El GL		77.316		0.567	1.00 60.32
ATOM					76.448	3 -3.378		1.00 62.17
ATOM			E2 GLU		78.371	-2.575		1.00 60.48
ATOM		_			79.151	0.658		1.00 43.27
ATOM		_			79.957	1.366		
ATOM		_			79.232	0.385		1.00 44.49
ATOM					80.374	0.799		1.00 43.29
ATOM	246				79.910			1.00 44.01
ATOM	246	_			81.381			1.00 42.35
	246	_		497	80.997			1.00 45.60
ATOM	246			498	82.666	-0.025		1.00 43.35
ATOM	2464			498	83.709	-1.042		1.00 48.78
ATOM	246!		3 ILE	498	84.611	-0.977	6.262	1.00 49.43
ATOM	2466			498	85.681	-2.054	5.014	1.00 50.66
ATOM	2467		I ILE	498	83.780	-1.150	5.082	1.00 51.85
ATOM	2468		)1 ILE	498	83.073	0.112	3.741	1.00 50.27
ATOM	2469		ILE	498	84.572	-0.878	3.255	1.00 54.24
ATOM	2470	0	ILE	498	85.055	0.219	7.510	1.00 50.32
ATOM	2471	N	GLY	499	84.713		7.801	1.00 49.08
ATOM	2472	CA	GLY	499	85.526	-1.964	8.270	1.00 51.88
ATOM	2473		GLY	499	85.061	~1.958		1.00 55.86
ATOM	2474	0	GLY	499	85.885	-1.111		1.00 59.72
ATOM	2475	N	LEU	500	83.747	-0.545		1.00 61.66
ATOM	2476	CA	LEU	500	83.167	-1.058		1.00 59.88
ATOM	2477	CB	LEU	500	81.663	-0.275		1.00 58.62
ATOM	2478	CG	LEU	500	80.764	-0.556		1.00 57.41
ATOM	2479	CD	LEU	500	79.331	-0.090		1.00 55.24
ATOM	2480		LEU	500		-0.536	11.168	1.00 51.91
ATOM	2481	С	LEU	500	80.845	1.426	10.799	1.00 54.93
ATOM	2482	0 -	LEU	500	83.849	-0.565	13.306	1.00 58.51
ATOM	2483	N	PRO	505	84.226	-1.710	13.576	00 60.71
ATOM	2484	CD	PRO	505	87.501	-6.102	10.460 1	00 82.25
ATOM	2485	CA	PRO		88.578	-6.722		.00 82.69
ATOM	2486	CB	PRO	505 505	87.860	-4.730		.00 80.47
ATOM	2487	CG	PRO	505	89.257	-4.557		.00 80.88
ATOM	2488	C		505	89.782	-5.960		.00 81.84
ATOM	2489	0	PRO	505	87.850	-4.508		.00 77.40
ATOM	2490	И	PRO	505	88.038	-3.391		.00 76.83
	2430	1//	ASN	506		-5.584		.00 74.91
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MOTA	2491	CA	ASN	506	87.572	-5.502	6.375	1.00 73.04
ATOM	2492	CB	ASN	506	88.632	-6.406	5.749	1.00 73.39
ATOM	2493	С	ASN	506	86.180	-5.938	5.929	1.00 71.75
ATOM	2494	0	ASN	506	85.918	-6.094	4.739	1.00 71.33
ATOM	2495	N	ARG	507	85.294	-6.124	6.905	1.00 69.66
ATOM	2496	CA	ARG	507	83.924	-6.534	6.638	1.00 66.59
ATOM	2497	CB	ARG	507	83.369	-7.329	7.819	1.00 69.86
ATOM	2498	С	ARG	507	83.048	-5.321	6.409	1.00 63.59
MOTA	2499	0	ARG	507	83.225	-4.291	7.070	1.00 64.09
ATOM	2500	N	VAL	508	82.126	-5.429	5.462	1.00 59.52
ATOM	2501	CA	VAL	508	81.217	-4.334	5.187	1.00 57.28
ATOM	2502	CB	LAV	508	80.905	-4.178	3.686	1.00 55.73
ATOM	2503		VAL	508	82.163	-3.952	2.922	1.00 57.01
ATOM	2504		VAL	508	80.184	-5.390	3.149	1.00 58.06
ATOM	2505	С	VAL	508	79. <b>9</b> 28	-4.614	5.935	1.00 57.10
ATOM	2506	0	VAL	508	79.483	-5 <b>.75</b> 9	6.018	1.00 57.35
MOTA	2507	N	THR	509	79.345	-3.555	6.482	1.00 55.31
MOTA	2508	CA	THR	509	78.107	-3.652	7.227	1.00 50.14
MOTA	250 <del>9</del>	CB	THR	509	78.329	-3.192	8.686	1.00 50.91
ATOM	2510	OG1		509	79.476	-3.851	9.227	1.00 49.20
ATOM	2511	CG2	THR	509	77.123	-3.524	9.559	1.00 51.96
ATOM	2512	C	THR	509	77.140	-2.705	6.528	1.00 47.53
ATOM	2513	0	THR	509	77.485	-1.558	6.242	1.00 47.22
ATOM	2514	N	LYS	510	75.958	-3.191	6.191	1.00 45.64
ATOM	2515	CA	LYS	510	74.975	-2.333	5.551	1.00 44.44
ATOM	2516	СВ	LYS	510	73.861	-3.175	4.948	1.00 46.74
ATOM	2517	CG	LYS	510	73.008	-2.420	3.950	1.00 54.51
ATOM	2518	CD	LYS	510	73.463	-2.645	2.513	1.00 54.97
ATOM	2519	CE	LYS	510	72.846	-3.917	1.934	1.00 58.25
ATOM	2520	NZ	LYS	510	73.112	-5.150	2.740	1.00 58.33
ATOM .	2521	C	LYS	510	74.430	-1.470	6.696	1.00 42.75
MOTA	2522	0	LYS	510	74.053	-2.006	7.742	1.00 43.14
ATOM	2523	N	VAL	511	74.443	-0.149	6.531	1.00 38.63
ATOM	2524	CA	VAL	511	73.975	0.757	7.576	1.00 34.16
ATOM ATOM	2525 2526	CB	VAL	511	75.161	1.399	8.333	1.00 35.66
ATOM		CG1	VAL	511	75.922	0.340	9.100	1.00 31.46
ATOM	2527 2528	CG2 C	VAL VAL	511 511	76.098	2.100	7.357	1.00 35.08
ATOM	2529	0	VAL	511	73.116	1.873	7.024	1.00 31.58
ATOM	2530	N	ALA	512	72.962 72.542	1.984 2.687	5.818	1.00 33.18
ATOM	2531	CA	ALA	512	71.724		7.906	1.00 30.77
ATOM	2532	CB	ALA	512	70.382	3.818 3.774	7.484 8.145	1.00 28.58
ATOM	2533	C	ALA	512	72.487	5.075		1.00 26.09
ATOM	2534	0	ALA	512	72.996		7.905	1.00 29.94
ATOM	2535	N	VAL	513		5.151 6.057	9.031	1.00 29.90
ATOM	2536	CA	VAL	513	72.556 73.286	7.290	7.012	1.00 28.68
ATOM	2537	CB	VAL	513	74.439	7.503	7.280 6.269	1.00 28.26
ATOM	2538	CG1		513	75.213	8. <b>7</b> 30	6.618	1.00 26.92
ATOM	2539	CG2		513	75.213	6.308	6.238	1.00 25.26
MOTA	2540	C	VAL	513	72.383	8.526	7.230	1.00 25.10 1.00 29.54
ATOM	2541	0	VAL -	513	71.745	8.799	6.200	1.00 29.54
ATOM	2542	N	LYS	514	72.304	9.228	8.359	1.00 28.94
	~~ ~ ~ ~	••		~ 1 4	.2.307	J. 240	0.337	4.00 ∠8.94

ATO		<b>54</b> 3	CA	LYS	514	71.5	10	70.45	_				
ATO.		44	CB	LYS	514	70.9		10.45		_		28.60	
ATO		45	CG	LYS	514	69.9		10.61			.00	31.19	9
ATO		46	CD	LYS	514	69.4		9.54			.00	31.41	1
ATO		47	CE	LYS	514	68.4		9.92		_	.00	40.14	1
ATON			NZ	LYS	514	67.1		8.89			.00	48.93	3
ATON		49	C	LYS	514	72.4		8.86			. 00	57.07	,
ATOM		50	0	LYS	514	73.5		11.636			00	25.53	j
ATOM		51	N	MET	515	71.92		11.714			00	20.42	
ATOM		52	CA	MET	515	72.6		12.576				26.63	
ATOM			CB	MET	515	73.42		13.762				27.59	
ATOM			CG 1	MET	515	72.50		13.487	_		00	28.22	
ATOM			SD I	MET	515	73.37		13.026			00	28.70	
ATOM			CE P	1ET	515	73.94		12.418		.3 1.	00	32.30	
ATOM				/ET	515	71.68		10.803	3.71		00 :	24.88	
ATOM	255	_	Ŋ	1ET	515	70.47		14.880	6.77	9 1.	00 2	28.41	
ATOM	255	9 N	I	ΈU	516	72.20		14.685	6.88	9 1.	0 C	32.15	
ATOM	256	0 C	'A L	EU	516			16.056	6.46	6 1.6	00 2	29.12	
ATOM	256	1 C	B L	EU	516	71.38		17.220	6.18	0 1.0	00 2	29.98	
ATOM	256	2 C	G L	EU	516	72.11		18.512	6.59	3 1.0		5.32	
ATOM	256	3 C	D1 L		516	72.45		18.767	8.06			6.60	
ATOM	2564			EU	516	73.210		20.057	8.19	1.0	0 2	4.56	
ATOM	2565	5 C		EU	516	71.217		18.844	8.900	1.0	0 2	2.75	
ATOM	2566			EU	516	71.092		17.274	4.674	1.0	0 3	1.50	
ATOM	2567	N	L	YS	517	71.763		16.636	3.873			2.97	
ATOM	2568			ZS.	517	70.069		18.018	4.293	1.0	0 3	3.29	
ATOM	2569		3 Ly	rs	517	69.755		8.187	2.890	1.0	0 3:	2.20	
ATOM	2570	CG			517	68.246		.8.363	2.699	T.0	0 36	5.34	
ATOM	2571	CI			517	67.432		7.182	3.192	1.0	0 43	3.49	
A'TOM	2572	CE			517	66.172		6.940	2.356	1.00	53	3.91	
ATOM	2573	NZ			517	65.088		7.984	2.581	1.00	58	3.71	
MOTA	2574	C	LY		517	63.902		7.740	1.704	1.00			
ATOM	2575	0	LY		517	70.520 70.917		9.455	2.507	1.00	31	.31	
ATOM	2576	N	SE		518	70.744		0.217	3.383	1.00	28	. 74	
ATOM	2577	CA	SE		518	70.744		9.672	1.213	1.00	32	.48	
MOTA	2578	CB	SE		518	71.486		0.840	0.714	1.00	33	. 52	
ATOM	2579	OG	SE	_	518	70.375		0.772	-0.809	1.00	32	. 98	
MOTA	2580	C	SE	_	518	70.896		0.407	-1.396	1.00	36	. 75	
MOTA	2581	0	SEI	_	518	71.580		2.189	1.110	1.00		. 62	
ATOM	2582	N	ASI		519	69.624		3.214	1.05B	1.00	34	. 57	
ATOM	2583	CA	ASI		519	68.943		2.193	1.485	1.00	35.	. 47	
ATOM	2584	CB	ASI		19	67.529		.422	1.885	1.00	36.	.10	
ATOM	2585	CG	ASF		19	66.668		.480	1.268	1.00	38.	.11	
ATOM	2586	OD1	ASP		19	67.150		.258	1.608	1.00	41.	64	
MOTA	2587		ASP		19	65.478		.309	2.253	1.00	41.	70	
ATOM	2588	C	ASP		19			.250	1.220	1.00			
MOTA	2589	0	ASP		19	68.881		. 645	3.395	1.00	34.	66	
ATOM	2590	N	ALA		20	68.266		.602	3.860	1.00	33.	39	
	2591	CA	ALA		20	69.551		.784	4.150	1.00	33.	52	
MOTA	2592	СВ	ALA		20	69.561		. 895	5.605	1.00	32.	12	
	2593	С	ALA		20	70.253		.687	6.207	1.00	32.	08	
	2594	0	ALA		20	70.242			6.076	1.00	30.	91	
				J.		71.014	24	778	5.331	1.00	30.	- 5 <b>7</b>	

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ATOM	2595	N	THR	521	69.943	24.555	7.311	1.00	30.80
MOTA	2596	CA	THR	521	70.546	25.738	7.921	1.00	32.33
MOTA	2597	CB	THR	521	69.493	26.763	8.440	1.00	34.30
ATOM	2598	OG1	THR	521	68.817	26.242	9.598	1.00	35.14
MOTA	2599	CG2	THR	521	68.484	27.109	7.366	1.00	37.70
MOTA	2600	C	THR	521	71.418	25.312	9.098	1.00	33.11
ATOM	2601	0	THR	521	71.518	24.125	9.426	1.00	31.39
ATOM	2602	N	GLU	522	72.022	26.293	9.753	1.00	34.91
ATOM	2603	CA	GLU	522	72.882	26.048	10.901	1.00	39.44
MOTA	2604	CB	GLU	522	73.516	27.357	11.360	1.00	46.96
ATOM	2605	CG	GLU	522	74.550	27.220	12.488	1.00	59.20
ATOM	2606	CD	GLU	522	75.919	26.740	12.011	1.00	64.70
MOTA	2607	OEl	GLU	522	76.910	27.478	12.219	1.00	63.87
MOTA	2608	OE2	GLU	522	76.006	25.627	11.445	1.00	71.55
MOTA	2609	С	GLU	522	72.083	25.428	12.044	1.00	39.61
MOTA	2610	0	GLU	522	72.587	24.554	12.757	1.00	36.74
ATOM	2611	N	LYS	523	70.827	25.849	12.193	1.00	38.60
ATOM	2612	CA	LYS	523	69.970	25.327	13.252	1.00	37.77
ATOM	2613	CB	LYS	523	68.628	26.053	13.273	1.00	44.52
ATOM	2614	CG	LYS	523	67.665	25.562	14.355	1.00	51.14
ATOM	2615	CD	LYS	523	66.380	24.983	13.756	1.00	57.39
MOTA	2616	CE	LYS	523	65.499	24.376	14.852	1.00	59.17
ATOM	2617	NZ	LYS	523	64.365	23.553	14.327	1.00	62.68
ATOM	2618	С	LYS	523	69.751	23.849	13.002	1.00	34.63
ATOM	2619	0	LYS	523	69.817	23.041	13.931	1.00	35.00
ATOM	2620	N	ASP	524	69.496	23.495	11.746	1.00	31.60
ATOM	2621	CA	ASP	524	69.293	22.100	11.367	1.00	29.05
MOTA	2622	CB	ASP	524	69.002	21.975	9.871	1.00	29.60
MOTA	2623	CG	ASP	524	67.695	22.626	9.472	1.00	31.90
ATOM	2624	OD1	ASP	524	66.666	22.368	10.130	1.00	38.83
ATOM	2625		ASP	524	67.687	23.383	8.485	1.00	29.79
ATOM	2626	С	ASP	524	70.558	21.317	11.696	1.00	28.02
ATOM	2627	0	ASP	524	70.494°	20.201	12.212	1.00	28.12
MOTA	2628	N	LEU	525	71.709	21.899	11.378	1.00	28.32
ATOM	2629	CA	LEU	525	72.971	21.231	11.677	1.00	27.71
ATOM	2630	CB	LEU	525	74.173	22.085	11.257	1.00	22.53
MOTA	2631	CG	LEU	525	75.548	21.490	11.602	1.00	22.13
ATOM	2632		LEU	525	75.677	20.082	11.019		19.92
ATOM	2633		LEU	525	76.673	22.401	11.147	1.00	18.60
ATOM	2634	C	LEU	525	73.007	20.952	13.162	1.00	27.44
ATOM	2635	0	LEU	525	73.227	19.817	13.577	1.00	29.73
ATOM	2636	N	SER	526	72.689	21.976	13.947	1.00	
MOTA	2637	CA	SER	526	72.672	21.891	15.412	1.00	30.83
MOTA	2638	CB	SER	526	72.222	23.230	16.006	1.00	
ATOM	2639	OG	SER	526	71.966	23.147	17.397	1.00	40.67
ATOM	2640	С	SER	526	71.765	20.777	15.931	1.00	29.32
ATOM	2641	0	SER	526	72.055	20.133	16.954	1.00	
ATOM	2642	N	ASP	527	70.644	20.587	15.242	1.00	
ATOM	2643	CA	ASP	527	69.681	19.558	15.601	1.00	
ATOM	2644	CB	ASP	527	68.392	19.798	14.829	1.00	
ATOM	2645	CG	ASP	527	67.640	21.052	15.290	1.00	29.22
MOTA	2646	OD1	ASP	527	68.016	21.662	16.320	1.00	26.80

3.000								
ATO		47	OD2 A	SP 527	66.6	60 21	.425 14.6	505 3 00 -
ATO		48		SP 527				
ATO		49	O A	SP 527				
ATO			N L	EU 528	70.8			-100 20.30
ATO			CA L	EU 528	71.4			
ATO		_		EU 528	71.9			
ATO				EU 528	72.4			
ATON			CD1 L		71.46			0
ATON			CD2 L	EU 528	72.72			
MOTA			C LE	EU 528	72.58			
ATOM	_		) LE	U 528	72.68			
ATOM		-	1 II	E 529	73.39			0.05
ATOM	_		CA IL	E 529	74.50			
ATOM		_	B IL	E 529	75.39			=
ATOM			G2 IL	E 529	76.54			
ATOM			G1 IL	E 529	75.96			
ATOM		-	D1 IL	E 529	76.98			
ATOM	-	_	'IL	E 529	73.95			
ATOM	266	5 0	IL		74.43			
ATOM	266	6 N	SE		72.91			
MOTA	266	7 C.	A SE	₹ 530	72.315		_	
ATOM	2668		B SEF	₹ 530	71.176			
ATOM	2669	9 00	G SEF	530	70.266			0.71
ATOM	2670	_	SER	530	71.795			00
ATOM	2671	0	SER		71.921			0
ATOM	2672	N	GLU		71.185			
ATOM	2673	CA	GLU		70.671			- 1 - 1 - 1 - 1 - 1
ATOM	2674		GLU		69.923			
ATOM	2675	CG	GLU		69.434			
MOTA	2676	CD	GLU		68.717			
MOTA	2677	OE	1 GLU	531	68.293	12.04		
ATOM	2678	OE	2 GLU	531	68.571	10.89		
ATOM	2679	С	GLU	531	71.765	12.94		
ATOM	2680	0	GLU	531	71.604	12.92	. –	
ATOM	2681	N	MET	532	72.851	11.98		
MOTA	2682	CA	MET	532	74.000	13.07		
MOTA	2683	CB	MET	532	75.073	12.15	-	1.00 28.35
MOTA	2684	CG	MET	532	76.458	12.63		1.00 29.48
ATOM	2685	SD	MET	532	77.650	12.03		1.00 25.84
MOTA	2686	CE	MET	532	77.831	12.69		1.00 30.60
MOTA	2687	С	MET	532	74.571	14.37		1.00 20.10
MOTA	2688	0	MET	532	74.876	12.120		1.00 29.06
ATOM	2689	N	GLU	533	74.640	11.053		1.00 28.22
ATOM	2690	CA	GLU	533	75.150	13.289		1.00 28.61
ATOM	2691	CB	GLU	533		13.388		1.00 28.40
ATOM	2692	CG	GLU	533	75.340	14.846		1.00 29.34
ATOM	2693	CD	GLU	533	76.449	15.534		1.00 31.87
ATOM	2694		GLU	533	77.822	14.923		1.00 35.10
ATOM	2695	OE2		533	78.242	14.831		1.00 37.36
ATOM	2696	C	GLU	533	78.490	14.543		1.00 37.71
ATOM	2697	0	GLU		74.211	12.684	_	1.00 31.03
ATOM	2698	N	MET	533 534	74.651	11.936	22.906	1.00 30.76
			· ···· +	534	72.909	12.902	21.860	1.00 31.71



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ATOM	2699	CA	MET	534	71.940	12.256	22.727	1.00 30.58
ATOM	2700	CB	MET	534	70.510	12.620	22.315	1.00 33.53
ATOM	2701	CG	MET	534	69.538	12.624	23.509	0.50 32.45
ATOM	2702	SD	MET	534	67.778	12.682	23.150	0.50 30.95
ATOM	2703	CE	MET	534	67.523	14.422	22.895	0.50 30.50
ATOM	2704	С	MET	534	72.158	10.752	22.616	1.00 28,44
ATOM	2705	0	MET	534	72.304	10.077	23.614	1.00 27.63
ATOM	2706	N	MET	535	72.216	10.232	21.395	1.00 30.00
ATOM	2707	CA	MET	535	72.448	8.800	21.176	1.00 29.38
MOTA	2708	CB	MET	535	72.626	8.483	19.690	1.00 25.41
MOTA	2709	CG	MET	535	71.395	8.753	18.893	1.00 25.06
ATOM	2710	SD	MET	535	71.468	7.917	17.344	1.00 27.17
ATOM	2711	CE	MET	535	71.439	9.227	16.247	1.00 33.70
MOTA	2712	C	MET	535	73.675	8.345	21.938	1.00 30.77
MOTA	2713	0	MET	535	73.681	7.254	22.534	1.00 27.49
MOTA	2714	N	LYS	536	74.710	9.183	21.916	1.00 32.72
ATOM	2715	CA	LYS	536	75.937	8.889	22.649	1.00 34.05
ATOM	2716	CB	LYS	536	76.995	9.964	22.401	1.00 32.69
ATOM	2717	CG	LYS	536	77.719	9.838	21.073	1.00 28.00
ATOM	2718	CD	LYS	536	78.732	10.956	20.941	1.00 29.61
ATOM	2719	CE	LYS	536	79.242	11.124	19.514	1.00 26.58
ATOM	2720	NZ	LYS	536	80.020	12.389	19.460	1.00 22.22
ATOM	2721	C	LYS	536	75.652	8.769	24.145	1.00 34.80
ATOM	2722	0	LYS	536	76.004	7.763	24.750	1.00 34.44
ATOM	2723	N	MET	537	74.958	9.749	24.716	1.00 34.66
MOTA	2724	CA	MET	537	74.634	9.724	26.131	1.00 37.25
ATOM	2725	CB	MET	537	73.951	11.034	26.549	1.00 46.08
ATOM	2726	CG	MET	537	74.862	12.272	26.619	1.00 57.95
ATOM	2727	SD	MET	537	76.159	12.203	27.919	1.00 66.50
MOTA	2728	CE	MET	537	75.287	12.873	29.377	1.00 64.52
ATOM	2729	C	MET	537	73.749	8.537	26.523	1.00 36.05
MOTA	2730	0	MET	537	74.021	7.865	27.514	1.00 36.71
MOTA	2731	N	ILE	538	72.730	8.255	25.719	1.00 33.77
MOTA	2732	CA	ILE	538	71.804	7.160	26.007	1.00 30.52
MOTA	2733	CB	ILE	538	70.616	7.172	25.012	1.00 28.15
MOTA	2734	CG2	ILE	538	69.780	5.899	25.122	1.00 26.08
ATOM	2735	CG1	ILE	538	69.729	8.377	25.289	1.00 26.24
ATOM	2736	CD1	ILE	538	68.644	8.558	24.256	1.00 26.87
MOTA	2737	С	ILE	538	72.399	5.750	26.100	1.00 30.05
ATOM	2738	0	ILE	538	71.984	4.950	26.941	1.00 31.57
ATOM	2739	N	GLY	539	73.320	5.424	25.211	1.00 30.34
MOTA	2740	CA	GLY	539	73.910	4.103	25.249	1.00 28.22
ATOM	2741	C	GLY	539	73.158	3.094	24.408	1.00 31.25
ATOM	2742	0	GLY	539	72.050	3.359	23.935	1.00 32.88
ATOM	2743	N	LYS	540	73.781	1.933	24.221	1.00 31.96
ATOM	2744	CA	LYS	540	73.222	0.845	23.416	1.00 33.40
ATOM	2745	CB	LYS	540	74.342	-0.023	22.878	1.00 31.53
MOTA	2746	CG	LYS	540	75.177	0.645	21.846	1.00 37.05
ATOM	2747	CD	LYS	540	76.273	-0.266	21.361	1.00 40.15
ATOM	2748	CE	LYS	540	77.143	0.480	20.363	1.00 46.84
ATOM	2749	NZ	LYS	540	76.374	0.920	19.152	1.00 48.60
ATOM	2750	С	LYS	540	72.183	-0.090	24.023	1.00 36.22

ATO	M 275	:1 /						
ATO		`			72.23	7 -0.430	25.215	1.00 40.10
ATO			V HIS		71.254	-0.521	23.175	
ATO			CA HIS		70.223	-1.486	23.535	
ATO	- · <del>-</del>		B HIS		69.064	-0.860		
MOTA			G HIS		68.127	-1.862		
			D2 HIS		68.127			1.00 32.39
ATOM	- · <del>-</del>		D1 HIS		67.086	-2.411		1.00 32.39
ATOM			E1 HIS		66.489	-3.329		1.00 33.35
ATOM	_		E2 HIS	541	67.096			
ATOM	_		HIS	541	69.720		22.275	1.00 30.46
ATOM			HIS	541	69.648		21.200	1.00 35 33
ATOM			LYS	542	69.348	-3.478	22.430	1.00 34.87
ATOM		3 C	A LYS	542	68.908	-4.311	21.306	1.00 35.42
ATOM	•		3 LYS	542	68.715	-5.766	21.753	1.00 32.02
ATOM			LYS	542	67.652	-3.848	20.614	1.00 30.96
MOTA	2766	5 0	LYS	542	67.474	-4.058	19.417	1.00 30.02
ATOM	2767	7 N	ASN	543	66.778	-3.212	21.369	1.00 29.10
ATOM	2768	C.F	ASN	543	65.529	-2.754		1.00 28.54
ATOM	2769	CE	ASN	543	64.372	-3.241	20.803	1.00 28.20
ATOM	2770	CG	ASN	543	64.387	-4.739	21.660	1.00 29.73
ATOM	2771	OD	1 ASN	543	64.732	-5.242	21.840	1.00 30.74
ATOM	2772	ND	2 ASN	543	64.053	-5.462	22.909	1.00 32.96
ATOM	2773	C	ASN	543	65.426	-1.257	20.787	1.00 29.58
ATOM	2774	0	ASN	543	64.342	-0.679	20.529	1.00 28.06
MOTA	2775	N	ILE	544	66.546	-0.635	20.647	1.00 28.86
ATOM	2776	CA	ILE	544	66.582		20.168	1.00 26.70
ATOM	2777	CB	ILE	544	67.052	0.794	19.833	1.00 26.81
ATOM	2778	CG	2 ILE	544	66.338	1.721	21.019	1.00 24.75
ATOM	2779	CG		544	68.568	1.353	22.306	1.00 20.02
ATOM	2780	CD:		544	69.105	1.614	21.234	1.00 23.73
ATOM	2781	C	ILE	544	67.582	2.531	22.332	1.00 21.64
MOTA	2782	0	ILE	544	68.388	0.901	18.680	1.00 27.95
ATOM	2783	N	ILE	545	67.449	-0.008	18.480	1.00 26.80
ATOM	2784	CA	ILE	545	68.376	1.940	17.849	1.00 29.22
ATOM	2785	СВ	ILE	545	67.824	2.163	16.745	1.00 27.14
ATOM	2786	CG2		545	68.920	3.164		1.00 26.10
ATOM	2787	CG1	_	545		3.556		1.00 24.70
ATOM	2788	CD1		545	66.625	2.568		1.00 23.78
ATOM	2789	С	ILE	545	66.988			1.00 22.15
ATOM	2790	0	ILE	545	69.631			1.00 28.14
MOTA	2791	N	ASN	546	69.586			1.00 28.21
ATOM	2792	CA	ASN	546	70.740	_		1.00 28.40
ATOM	2793	СВ	ASN	546	72.004			1.00 28.49
ATOM	2794	CG	ASN	546	72.709			1.00 27.05
ATOM	2795		ASN	546	71.956		19.470	1.00 27.29
ATOM	2796		ASN		71.793		20.540	L.00 29.92
ATOM	2797	C	ASN	546 546			19.235	L.00 24.63
ATOM	2798	0		546	72.982			1.00 28.39
ATOM	2799	N	ASN	546	73.045			.00 29.62
ATOM	2800	CA	LEU	547	73.774	3.982	17.579 1	00 29.91
ATOM	2801	CB	LEU	547	74.828	4.750		.00 30.68
ATOM	2802	CG	LEU	547	75.297			00 25.28
	2002	<b>C</b> G	LEU	547	76.367	6.828	L7.267 1	.00 24.81

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MOTA	2803	CD1	LEU	547	75.868	7.524	15.990	1.00 22.25
ATOM	2804	CD2	LEU	547	76.716	7.853	18.313	1.00 24.17
MOTA	2805	С	LEU	547	76.016	3.812	16.629	1.00 31.67
ATOM	2806	0	LEU	547	76.481	3.090	17.509	1.00 31.34
ATOM	2807	N	LEU	548	76.475	3.823	15.380	1.00 30.60
ATOM	2808	CA	LEU	548	77.594	2.995	14.955	1.00 29.31
MOTA	2809	CB	LEU	548	77.197	2.165	13.729	1.00 25.94
ATOM	2810	CG	LEU	548	75.968	1.247	13.883	1.00 28.78
MOTA	2811	CD1	LEU	548	75.848	0.360	12.659	1.00 27.14
MOTA	2812	CD2	LEU	548	76.049	0.392	15.149	1.00 23.72
MOTA	2813	C	LEU	548	78.850	3.821	14.644	1.00 31.60
MOTA	2814	0	LEU	548	79.967	3.330	14.753	1.00 32.65
ATOM	2815	N	GLY	549	78.665	5.076	14.248	1.00 32.22
ATOM	2816	CA	GLY	549	79.795	5.928	13.937	1.00 31.40
ATOM	2817	C	GLY	549	79.344	7.267	13.391	1.00 30.78
ATOM	2818	0	GLY	549	78.140	7.536	13.291	1.00 29.84
ATOM	2819	N	ALA	550	80.320	8.099	13.045	1.00 31.88
ATOM	2820	CA	ALA	550	80.073	9.416	12.485	1.00 30.14
ATOM	2821	CB	ALA	550	79.634	10.382	13.590	1.00 31.08
ATOM	2822	C	ALA	550	81.291	9.978	11.742	1.00 28.78
ATOM	2823	0	ALA	550	82.447	9.705	12.102	1.00 26.39
ATOM	2824	N	CYS	551	81.011	10.690	10.651	1.00 28.48
ATOM	2825	CA	CYS	551	82.012	11.391	9.846	1.00 23.69
ATOM	2826	CB	CYS	551	81.825	11.128	8.352	1.00 24.18
ATOM	2827	SG	CYS	551	81.870	9.395	7.840	1.00 28.40
ATOM	2828	C	CYS	551	81.612	12.847	10.127	1.00 20.99
ATOM	2829	0	CYS	551	80.561	13.282	9.684	1.00 22.11
ATOM	2830	N	THR	552	82.357	13.524	10.996	1.00 20.18
MOTA	2831	CA	THR	552	82.073	14.914	11.349	1.00 22.79
MOTA	2832	CB	THR	552	82.090	15.080	12.874	1.00 23.16
ATOM	2833	OG1		552	83.408	14.803	13.363	1.00 23.52
MOTA	2834		THR	552	81.125	14.112	13.529	1.00 25.31
MOTA MOTA	2835	C	THR	552	83.138	15.886	10.824	1.00 24.74
ATOM	2836 2837	O N	THR	552 553	82.939	17.103	10.782	1.00 22.75
ATOM	2838	CA	GLN GLN	553 553	84.276	15.334	10.431	1.00 26.82
MOTA	2839	CB	GLN	553	85.387 86.686	16.153	9.980	1.00 26.99
ATOM	2840	CG	GLN	553	86.632	15.627 15.494	10.602 12.141	1.00 26.40
ATOM	2841	CD	GLN	553	86.438			1.00 22.69
ATOM	2842		GLN	553	87.259	16.836 17.729	12.823	1.00 25.90
ATOM	2843		GLN	553	85.351	16.994	12.656 13.566	1.00 29.03 1.00 23.53
ATOM	2844	C	GLN	553	85.502	16.216	8.466	1.00 23.33
ATOM	2845	o	GLN	553	85.177	15.259	7.779	1.00 20.23
ATOM	2846	N	ASP	554	85.863	17.394	7.968	1.00 30.00
ATOM	2847	CA	ASP	554	86.084	17.631	6.531	1.00 28.38
ATOM	2848	CB	ASP	554	87.410	17.031	6.105	1.00 26.38
ATOM	2849	CG	ASP	554	88.538	17.570	6.912	1.00 26.78
ATOM	2850		ASP	554	88.789	18.795	6.823	1.00 31.33
ATOM	2851		ASP	554	89.141	16.795	7.665	1.00 35.18
ATOM	2852	C	ASP	554	85.011	17.221	5.545	1.00 29.04
ATOM	2853	0	ASP	554	85.278	16.468	4.610	1.00 29.14
ATOM	2854	N	GLY	555	83.824	17.793	5.709	1.00 31.22
					03.024	~,	3.709	1.00 J1.20



ATO			CA G	LY 555	82.723	3 17.49	0 4 03 :	
ATO		56	C GI	LY 555	81.446			
OTA		57	O GI	Y 555	81.448			
ATON		58	N PF	8O 556	80.317			
ATOM	1 289	59	CD PR		80.213			
ATOM	1 286	50 (	CA PR		79.010			
ATOM	1 286	51 (	CB PR					1.00 25.11
ATOM	286		CG PR		78.107			
ATOM					79.077			
ATOM					79.006			1.00 27.67
ATOM					79.676	14.947		1.00 27.13
ATOM		_	A LE		78.253	16.297		1.00 29.27
ATOM		_ `	B LE		78.164	15.405		1.00 31.19
ATOM			G LE		77.583	16.130	10.188	1.00 29.94
ATOM	286				77.019	15.260	11.323	1.00 26.87
ATOM	287	_	D1 LE		78.131	14.540		1.00 23.83
ATOM	287		D2 LEU		76.237	16.146	12.275	1.00 23.80
ATOM					77.291	14.193	8.651	1.00 31.97
ATOM	287	_			76.158	14.332	8.184	1.00 31.97
ATOM	2873				77.857	13.010	8.882	
ATOM	2874				77.145	11.767	8.664	1.00 31.12
	2875				77.905	10.869	7.694	1.00 28.86
ATOM	2876				78.017	11.395	6.281	1.00 28.58
ATOM	2877		Ol TYR		79.034	10.962	5.443	1.00 32.33
MOTA	2878		El TYR	558	79.161	11.447		1.00 35.23
ATOM	2879	CI	2 TYR	558	77.123	12.336	4.151	1.00 37.54
ATOM	2880	CE	2 TYR	558	77.248	12.832	5.787	1.00 35.27
ATOM	2881	CZ	TYR	558	78.276	12.382	4.493	1.00 36.43
ATOM	2882		TYR	558	78.423	12.869	3.680	1.00 37.05
ATOM	2883	С	TYR	558	77.000		2.394	1.00 39.97
ATOM	2884	0	TYR	558	77.985	11.071	10.004	1.00 26.63
MOTA	2885	N	VAL	<b>5</b> 59	75.756	10.885	10.725	1.00 24.67
ATOM	2886	CA	VAL	559	75.429	10.774	10.365	1.00 28.15
ATOM	2887	CB	VAL	559	74.262	10.070	11.610	1.00 27.70
MOTA	2888	CG:	1 VAL	559		10.770	12.372	1.00 26.63
ATOM	2889	CG:		559	73.876	9.959	13.603	1.00 24.70
ATOM	2890	С	VAL	559		12.186	12.792	1.00 26.71
ATOM	2891	0	VAL	559	75.061	8.635	11.205	1.00 27.08
ATOM	2892	N	ILE	560	73.965	8.357	10.710	1.00 25.39
ATOM	2893	CA	ILE	560	76.002	7.729	11.399	1.00 28.25
ATOM	2894	CB	ILE	560	75.820	6.335	11.000	1.00 29.62
ATOM	2895		ILE	560	77.225		10.678	1.00 30.06
ATOM	2896		ILE		77.045		10.101	1.00 31.58
ATOM	2897		ILE	560	78.004	6.557	9.686	1.00 27.50
ATOM	2898	C		560	79.492	6.239	9.629	1.00 23.31
ATOM	2899		ILE	560	75.075	5.488	,	1.00 29.88
ATOM	2900	0	ILE	560	75.586			23.33
ATOM		N	VAL	561	73.857			00 29.09
ATOM	2901	CA	VAL	561	73.053			.00 28.70
ATOM	2902	СВ	VAL	561	71.743			.00 25.29
	2903		VAL	561	72.072			
MOTA	2904		VAL	561	70.887			.00 22.91
ATOM	2905	C	VAL	561				.00 22.38
ATOM	2906	0	VAL	561				.00 27.99
						550 1	.0.783 1	.00 27.88

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ATOM	2907	N	GLU	562	72.143	1.969	12.754	1.00	27.38
ATOM	2908	CA	GLU	562	71.759	0.616	12.347	1.00	28.01
MOTA	2909	CB	GLU	562	71.246	-0.161	13.555	1.00	25.37
ATOM	2910	CG	GLU	562	72.322	-0.487	14.570	1.00	29.22
MOTA	2911	CD	GLU	562	71.785.	-1.190	15.796	1.00	30.94
MOTA	2912	OE1	GLU	562	72.440	-2.135	16.271	1.00	34.82
ATOM	2913	OE2	GLU	562	70.716	-0.795	16.297	1.00	32.77
MOTA	2914	С	GLU	562	70.695	0.610	11.266	1.00	29.83
ATOM	2915	0	GLU	562	69.822	1.452	11.274	1.00	34.69
MOTA	2916	N	TYR	563	70.755	-0.364	10.362	1.00	31.35
MOTA	2917	CA	TYR	563	69.806	-0.527	9.255	1.00	33.79
MOTA	2918	CB	TYR	563	70.586	-0.987	8.022	1.00	32.37
ATOM	2919	CG	TYR	563	69.759	-1.232	6.778	1.00	31.70
MOTA	2920	CD1	TYR	563	68.858	-0.277	6.319	1.00	35.00
MOTA	2921	CE1	TYR	563	68.101	-0.490	5.161	1.00	35.62
MOTA	2922	CD2	TYR	563	69.888	-2.416	6.053	1.00	31.64
MOTA	2923	CE2	TYR	563	69.138	-2.644	4.894	1.00	32.96
MOTA	2924	CZ	TYR	563	68.242	-1.674	4.462	1.00	36.20
MOTA	2925	OH	TYR	563	67.494	-1.906	3.340	1.00	39.54
ATOM	2926	C	TYR	563	68.668	-1.527	9.593	1.00	37.26
ATOM	2927	0	TYR	563	68.915	-2.566	10.212	1.00	38.86
ATOM	2928	N	ALA	564	67.428	-1.180	9.220	1.00	39.09
MOTA	2929	CA	ALA	564	66.256	-2.027	9.467	1.00	37.64
ATOM	2930	CB	ALA	564	65.290	-1.317	10.366		41.34
MOTA	2931	С	ALA	564	65.600	-2.337	8.124		39.33
ATOM	2932	0	ALA	564	64.700	-1.628	7.661	1.00	
ATOM	2933	N	SER	565	66.033	-3.432	7.515	1.00	
ATOM	2934	C'A	SER	565	65.567	-3.867	6.202	1.00	40.22
ATOM	2935	CB	SER	565	66.302	-5.133	5.808	1.00	38.50
ATOM	2936	OG	SER	565	66.174	-6.084	6.847	1.00	
ATOM	2937	C	SER	565	64.095	-4.087	5.987	1.00	
ATOM	2938	0	SER	565	63.657	-4.155	4.840	1.00	
ATOM	2939	N	LYS	566	63.322	-4.248	7.054	1.00	
MOTA	2940	CA	LYS	566	61.893	-4.462	6.883	1.00	
ATOM	2941	CB	LYS	566	61.455	-5.681	7.684	1.00	
MOTA	2942	CG	LYS	566	62.003	-6.977	7.088	1.00	
MOTA	2943	CD	LYS	566	61.929	-8.148	8.040	1.00	
ATOM	2944	CE	LYS	566	62.582	-9.362	7.426	1.00	
ATOM	2945	NZ	LYS	566		-10.465	8.417		59.37
ATOM	2946 2947	C	LYS	566	61.029	-3.234	7.143	1.00	
ATOM ATOM		0	LYS	566	59.815	-3.337	7.341	1.00	
ATOM	2948 2949	N	GLY	567	61.663	-2.061	7.100	1.00	
ATOM		CA	GLY	567	60.956	-0.808	7.291	1.00	
MOTA	2950	С	GLY	567	60.306	-0.640	8.644	1.00	
	2951	O	GLY	567	60.727	-1.265	9.614	1.00	
ATOM ATOM	2952 2953	N	ASN	568	59.296	0.218	8.711	1.00	
		CA	ASN	568	58.615	0.447	9.966	1.00	
ATOM ATOM	2954	CB	ASN	568	57.961	1.839	10.029	1.00	
	2955	CG	ASN	568	56.701	1.962	9.163	1.00	
ATOM	2956	OD1		568	55.718	1.241	9.338	1.00 4	
ATOM ATOM	2957	ND2		568	56.710	2.932	8.263	1.00	
ALON	2958	С	ASN	568	57.610	-0.657	10.269	1.00	88.91

ATO	M 29	59	O AS	N 500				
ATO					57.21		9.384	1.00 39.95
ATO		_			57.20		7 11.534	1.00 38.93
ATO					56.25		2 12.047	1.00 36.49
ATO					56.12	6 -1.507		
ATO			CG LE		55.15	0 -2.417		50.55
ATO			CD1 LE		55.55			1.00 31.86
			CD2 LE		55.14			
ATON			LE	J 569	54.87			
ATOM		-	LE	J 569	54.23			
ATOM			ARG	570	54.38			
ATOM		59 C	A ARG	570	53.06			1.00 36.63
ATOM			B ARG	570	52.73			1.00 36.68
ATOM		71 C	G ARG	570	51.33		10.188	1.00 37.76
ATOM	297	72 C	D ARG	570	51.21	_	9.623	1.00 46.41
ATOM	297	'3 N	E ARG		52.162		8.889	1.00 56.33
ATOM		4 C					7.779	1.00 63.05
ATOM	297		H1 ARG		53.010	- <del>-</del>	7.603	1.00 66.33
ATOM	297		H2 ARG		53.032		8.468	1.00 65.15
ATOM	297		ARG		53.853		6.580	1.00 66.56
ATOM	297	_	ARG		53.046		9.193	1.00 35.55
ATOM	297	_	GLU		52.248		9.018	1.00 35.33
ATOM	298			. –	53.978		8.320	1.00 37.20
ATOM	298			571	54.128		7.030	1.00 38.32
ATOM	2982			571	55.247	-0. <b>69</b> 5	6.261	1.00 40.15
ATOM	2983			571	55.001	0.803	6.152	1.00 49.09
ATOM				571	56.118	1.557	5.442	1.00 58.16
ATOM	2984		1 GLU	571	57.279	1.073	5.421	1.00 61.41
ATOM	2985			571	55.824	2.660	4.914	1.00 61.27
ATOM	2986		GLU	571	54.406	-2.906	7.170	1.00 36.74
ATOM	2987		GLU	571	53.863	-3.721	6.410	1.00 35.74
	2988		TYR	572	55.241	-3.266	8.141	
ATOM	2989			572	55.591	-4.665	8.401	1.00 35.13
ATOM	2990		TYR	572	56.591	-4.736	9.560	1.00 37.12
ATOM	2991		TYR	572	56.984	-6.128	10.029	1.00 34.39
MOTA	2992	CD	1 TYR	572	57.980	-6.869		1.00 33.48
ATOM	2993	CE:	_	572	58.394	-8.119		1.00 29.76
MOTA	2994	CD:	2 TYR	572	56.406	_		1.00 27.14
ATOM	2995	CE:	2 TYR	572	56.814			1.00 32.40
ATOM	2996	CZ	TYR	572	57.807			1.00 30.83
ATOM	2997	ОН	TYR	572	58.201			1.00 33.73
ATOM	2998	C	TYR	572	54.330			1.00 37.16
ATOM	2999	0	TYR	572	54.108	-5.468		1.00 38.92
ATOM	3000	N	LEU	573		-6.553		1.00 39.22
ATOM	3001	CA	LEU	573	53.507	-4.922	9.618	1.00 38.41
ATOM	3002	СВ	LEU		52.261		10.016	L.00 37.56
ATOM	3003	CG	LEU	573	51.573	-4.711	11.084	L.00 36.44
ATOM	3004		LEU	573 573	52.270	-4.617		1.00 33.91
ATOM	3005			573 573	51.555	-3.626		00 31.60
ATOM	3006		LEU	573	52.313			00 30.78
ATOM		С	LEU	573	51.315	-5.738		00 37.51
ATOM	3007	0	LEU	573	50.847	-6.836		.00 36.70
	3008	N	GLN	574	51.045	-4.643		.00 40.10
ATOM	3009	CA	GLN	574	50.141		6.986 1	00 41 40
ATOM	3010	CB	GLN	574	49.938			.00 41.10
						· <del>-</del>		.00 40.12

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ATOM	3011	CG	GLN	574	49.171	-2.381	7.374	1.00 40.77
MOTA	3012	CD	GLN	574	49.079	-0.987	6.852	1.00 43.90
ATOM	3013	OE1	GLN	574	49.679	-0.652	5.835	1.00 46.93
ATOM	3014	NE2	GLN	574	48.357		7.558	1.00 46.85
ATOM	3015	С	GLN	574	50.546	-5.638	5.875	1.00 41.31
ATOM	3016	0	GLN	574	49.699	-6.323	5.309	1.00 44.33
ATOM	3017	N	ALA	575	51.840	-5.735	5.601	1.00 41.46
ATOM	3018	CA	ALA	575	52.317	-6.628	4.555	1.00 39.80
ATOM	3019	CB	ALA	575	53.745	-6.301	4.218	1.00 40.58
MOTA	3020	C	ALA	575	52.197	-8.096	4.947	1.00 40.86
ATOM	3021	0	ALA	575	52.527	-8.975	4.165	1.00 41.50
ATOM	3022	N	ARG	576	51.757	-8.359	6.168	1.00 42.47
ATOM	3023	CA	ARG	576	51.624	-9.726	6.641	1.00 42.68
ATOM	3024	CB	ARG	576	52.679	-9.988	7.716	1.00 41.04
ATOM	3025	CG	ARG	576	54.095	-9.958	7.161	1.00 42.73
ATOM	3026	CD	ARG	576	55.156	-9.943	8.257	1.00 45.59
ATOM	3027	NE	ARG	576	56.514	-9.870	7.695	1.00 43.89
ATOM	3028	CZ	ARG	576	56.981	-8.856	6.969	1.00 43.35
ATOM	3029		ARG	576	56.219	-7.803	6.703	1.00 44.85
ATOM	3030		ARG	576	58.215	-8.902	6.497	1.00 41.84
ATOM	3031	C	ARG	576	50.232	-10.014	7.18C	1.00 44.86
ATOM	3032	0	ARG	576		-10.943	7.970	1.00 46.08
ATOM	3033	N	ARG	577	49.258	-9.216	6.753	1.00 46.72
ATOM	3034	C'A	ARG	577	47.877	-9.401	7.196	1.00 47.61
ATOM	3035	CB	ARG	577	46.994	-8.239	6.723	1.00 46.35
ATOM	3036	CG	ARG	577	47.101	-6.995	7.581	1.00 47.71
ATOM	3037	CD	ARG	577	46.329	-5.831	6.999	1.00 49.15
ATOM	3038	NE	ARG	577	46.213	-4.735	7.957	1.00 53.23
ATOM ATOM	3039	CZ	ARG	577	45.584	-3.587	7.725	1.00 54.38
ATOM	3040 3041	NH1		577	45.020	-3.368	6.549	1.00 56.41
ATOM	3041	NH2 C	ARG	577 577	45.481	-2.676	8.686	1.00 58.13
ATOM	3042	0	ARG	577		-10.740	6.743	1.00 47.36
ATOM	3044	N	GLN	594		-11.031 -13.948	5.550	1.00 48.52
ATOM	3045	CA	GLN	594		-14.067	7.960	1.00 68.05
ATOM	3046	CB	GLN	594		-15.220	8.772 8.277	1.00 66.75
ATOM	3047	C	GLN	594		-14.284	10.233	1.00 66.87
ATOM	3048	C	GLN	594		-15.264	10.580	1.00 64.71 1.00 64.86
ATOM	3049	N	LEU	595		-13.335	11.074	1.00 61.14
ATOM	3050	CA	LEU	595		-13.422	12.480	1.00 51.14
ATOM	3051	СВ	LEU	395		-12.008	13.056	1.00 56.33
ATOM	3052	CG	LEU	595		-11.147	12.203	1.00 57.36
ATOM	3053	CD1		595	53.375	-9.692	12.533	1.00 57.50
ATOM	3054	CD2		595		-11.598	12.382	1.00 56.98
ATOM	3055		LEU	595		-14.237	13.251	1.00 56.25
ATOM	3056		LEU	595		-14.359	12.834	1.00 56.60
ATOM	3057	N	SER	596		-14.845	14.341	1.00 53.07
ATOM	3058	CA	SER	596		-15.642	15.229	1.00 48.64
MOTA	3059	CB	SER	596		-16.841	15.736	1.00 46.41
ATOM	3060	OG	SER	596		-16.435	16.737	1.00 46.50
ATOM	3061	C	SER	596		-14.756	16.423	1.00 48.95
ATOM	3062	0	SER	596		-13.767	16.649	1.00 49.39

ATO		63	N :	SER	597	40.000
ATO		64		SER	597	19.033 213.163 17.242 1.00 50.27
ATO		65		SER	597	19.469 -14.387 18.424 1.00 51.93
ATO		66			597	48.391 -15.123 19.225 1.00 52.03
ATO		67	_		597	17.340 -15.854 18.365 1 00 F2 0F
ATO		68			597	50.665 -14.143 19.314 1.00 52.72
OTA	M 30	69			598	30.792 -13.093 19.943 1 00 FF 04
MOTA	4 30°	70			598	31.013 -15.100 19.344 1 00 53 55
MOTA					598	32.024 -14.961 20.159 1 00 53 6.
ATOM	1 30:			-	598	23.366 ~16.295 20.248 1 00 54 55
ATOM		73 (			98	21.576 -16.457 21.524 1.00 57.30
ATOM		74 (	_		98	33.03/ -1/.824 21.570 1 00 50 33
ATOM		_	_		98	33.700 -18.055 22.893 1.00 50 00
ATOM	307	6 (	L	_	98	24.040 -18.169 24.043 1 00 52 05
ATOM	307	7 (		_	98	33.720 -13.909 19.527 1 00 52 40
ATOM	307	8 N		_	99	34.273 -13.052 20.227 1 00 53 73
ATOM	307	_	'A AS	_	99	33.042 -13.960 18.198 1 00 50 55
MOTA	308		B AS	_	99	34.03/ -13.021 17.435 1.00 40 50
MOTA	308		G AS		99	34.300 -13.294 15.929 1.00 46 7-
ATOM	3082		D1 AS		99	33.233 -14.607 15.515 1 00 40 00
MOTA	3083		D2 AS	_	99	33.036 ~15.260 16.344 1 00 53 76
ATOM	3084		AS	_	99	55.100 -14.986 14.330 1 00 46 70
MOTA	3085	5 0				34.173 -11.598 17.706 1 00 40 66
ATOM	3086	N	LE			53.376 -10.703 17.960 1.00 52.86
ATOM	3087	, cz				52.652 -11.406 17.684 1.00 44.53
ATOM	3088	CE				52.272 -10.099 17.938 1.00 41.06
ATOM	3089					50.774 -10.100 17.632 1.00 39.23
ATOM	3090	CI	) LEC			10.334 -10.374 16.178 1.00 36.50
ATOM	3091	CD				51 000 0 202
ATOM	3092	C	LEU			52 542 0 625
ATOM	3093	0	LEU			52 890 2 45
ATOM	3094	N	VAL	60:	ı	52 417 10 555
ATOM	3095	CA	VAL			52 685 10 155
ATOM	3096	CB	VAL	601		52 236 11 222
ATOM	3097		1 VAL	601		52 254 10 555
ATOM	3098	CG:	2 VAL	601		50 040 77 05
ATOM	3099	C	VAL	601		54 192 0 00:
ATOM	3100	0	VAL	601		54 611 0 000
ATOM	3101	N	SER	602		54 986 -70 605
ATOM	3102	CA	SER	602		56 442 10 50
ATOM	3103	CB	SER	602		57 014 11 11 11 11 11 11 11 11 11 11 11 11 1
ATOM	3104	OG	SER	602		ED 434
ATOM	3105	C	SER	602		EC 050
ATOM	3106	0	SER	602		57 630 0 10-
ATOM	3107	N	CYS	603		56 330
ATOM	3108	CA	CYS	603		56 590 7 100 38,34
ATOM	3109	CB	CYS	603		55 715 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7
ATOM	3110	SG	CYS	603		55 735 5 1.00 38.09
ATOM	3111	С	CYS	603		56 202 6 222
	3112	0	CYS	603		57 039 5 309
	3113	N	ALA	604		55 100 6 700
ATOM	3114	CA	ALA	604		54 804 5 555
						34.804 -5.572 21.911 1.00 34.97

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ATOM	3115	CB	ALA	604	53.393	-5.917	22.409	1.00 34.13
ATOM	3116	С	ALA	604	55.791	-5.610	23.081	1.00 36.68
MOTA	3117	0	ALA	604	56.085	-4.585	23.704	1.00 36.78
MOTA	3118	N	TYR	605	56.281	-6.807	23.385	1.00 37.68
ATOM	3119	CA	TYR	605	57.254	-7.005	24.461	1.00 38.38
ATOM	3120	CB	TYR	605	57.533	-8.498	24.643	1.00 37.62
ATOM	3121	CG	TYR	605	58.635	-8.806	25.622	1.00 36.56
MOTA	3122	CD1	TYR	605	58.498	-8.509	26.974	1.00 39.05
MOTA	3123	CE1	TYR	605	59.520	-8.809	27.893	1.00 41.37
MOTA	3124	CD2	TYR	605	59.812	-9.407	25.198	1.00 38.09
MOTA	3125	CE2	TYR	605	60.848	-9.711	26.105	1.00 38.55
ATOM	3126	CZ	TYR	605	60.692	-9.409	27.454	1.00 40.73
ATOM	3127	ОН	TYR	605	61.707	-9.704	28.348	1.00 41.44
ATOM	3128	С	TYR	605	58.549	-6.267	24.123	1.00 38.44
MOTA	3129	0	TYR	605	59.053	-5.485	24.937	1.00 40.78
ATOM	3130	N	GLN	606	59.053	-6.501	22.908	1.00 36.07
ATOM	3131	CA	GLN	606	60.276	-5.872	22.398	1.00 35.28
ATOM	3132	CB	GLN	606	60.594	-6.415	21.002	1.00 34.24
ATOM	3133	CG	GLN	606	61.105	-7.851	21.005	1.00 32.26
ATOM	3134	CD	GLN	606	61.339	-8.388	19.608	1.00 30.17
ATOM	3135	OE1	GLN	606	62.274	-7.988	18.907	1.00 31.89
ATOM	3136	NE2	GLN	606	60.471	-9.285	19.182	1.00 30.68
MOTA	3137	С	GLN	606	60.210	-4.335	22.355	1.00 36.39
MOTA	3138	0	GLN	606	61.206	-3.660	22.632	1.00 39.59
MOTA	3139	N	VAL	607	59.040	-3.798	22.006	1.00 32.78
MOTA	3140	CA	VAL	607	58.839	-2.350	21.944	1.00 30.29
MOTA	3141	СВ	VAL	607	57.489	-1.982	21.221	1.00 28.48
ATOM	3142	CG1	VAL	607	57.219	-0.488	21.298	1.00 28.68
ATOM	3143	CG2	VAL	607	57.535	-2.416	19.742	1.00 22.96
ATOM	3144	С	VAL	607	58.868	-1.766	23.364	1.00 30.21
ATOM	3145	0	VAL	607	59.469	-0.705	23.591	1.00 31.24
ATOM	3146	N	ALA	608	58.224	-2.451	24.311	1.00 27.88
ATOM	3147	CA	ALA	608	58.187	-2.001	25.694	1.00 27.66
ATOM	3148	CB	ALA	608	57.242	-2.874	26.494	1.00 26.42
ATOM	3149	С	ALA	608	59.585	-2.019	26.309	1.00 29.04
MOTA	3150	0	ALA	608	59.950	-1.144	27.094	1.00 27.53
ATOM	3151	N	ARG	609	60.377	-3.013	25.932	1.00 28.91
ATOM	3152	CA	ARG	609	61.733	-3.120	26.440	1.00 31.64
MOTA	3153	CB	ARG	609	62.394	-4.405	25.953	1.00 33.78
ATOM	3154	CG	ARG	609	61.672	-5.647	26.373	1.00 38.53
ATOM	3155	CD	ARG	609	62.636	-6.791	26.448	1.00 41.78
MOTA	3156	NE	ARG	609	63.319	-6.838	27.733	1.00 47.58
MOTA	3157	CZ	ARG	609	64.441	-7.510	27.955	1.00 51.52
MOTA	3158	NH1	ARG	609	65.012	-8.179	26.964	1.00 50.61
MOTA	3159	NH2	ARG	609	64.954	-7.569	29.186	1.00 54.36
MOTA	3160	C	ARG	609	62.581	-1.918	26.024	1.00 33.26
MOTA	3161	0	ARG	609	63.144	-1.221	26.885	1.00 34.50
ATOM	3162	N	GLY	610	62.624	-1.650	24.717	1.00 30.25
ATOM	3163	CA	GLY	610	63.395	-0.534	24.199	1.00 25.40
ATOM	3164	С	GLY	610	63.010	0.730	24.930	1.00 24.12
ATOM	3165	0	GLY	610	63.857	1.507	25.345	1.00 24.74
ATOM	3166	N	MET	611	61.712	0.907	25.131	1.00 25.81



n m	014								
AT	~	167	CA	MET	611	61.19	92 2 (	062 25.	
ATO		168	CB	MET	611	59.6			
AT(		169	CG	MET	611	59.21			
ATC		170		MET	611	59.97			
ATC	- '	171		MET	611	59.54			,
ATC ATC		172		MET	611	61.60			· • •
ATO		L73	0	MET	611	61.89			
ATO		74		GLU	612	61.56			
ATO		.75		GLU	612	61.95			
ATO		76		SLU	612	61.80			
ATO	- <del>-</del>	77		LU	612	62.38			
ATO	- <del>-</del>		CD G	LU	612	62.39			
ATO			OEl G		612	62.599			
ATON			OE2 G		612	62.226			
ATON				LU	612	63.409			
ATOM				LU	612	63.791			
MOTA	_			YR	613	64.196			
ATOM	,	`		YR	613	65.601			005
ATOM				YR	613	66.328			
ATOM				YR 	613	67.801			
ATOM		_	DI T		613	68.734			
ATOM		-	El T		613	70.090	0.64		
ATOM			D2 TY		613	68.252	1.909		
ATOM	319		E2 TY		613	69.596	2.306		
ATOM	319				613	70.512	1.674		
ATOM	319				613	71.826	2.089		
ATOM	319				613	65.724	2.760		
ATOM	319	_	TY		613	66.362	3.414		
ATOM	3196		A LE		614	65.081	3.326		
ATOM	3197				614	65.156	4.766	26.988	
MOTA	3198				614	64.314	5.157	25.781	1.00 31.88
ATOM	3199		)1 LET		614	64.760	4.601		
ATOM	3200		)2 LE(	_	614	63.783	5.016	23.346	1.00 29.19
ATOM	3201		LEU		614 614	66.134	5.133	24.111	1.00 32.49
ATOM	3202		LEU		614 614	64.698	5.538	28.218	1.00 36.38
ATOM	3203	-	ALA		614 615	65.325	6.525	28.618	1.00 33.81
ATOM	3204				615	63.608	5.076	28.821	1.00 38.08
ATOM	3205	СВ			615 615	63.066	5.711	30.018	1.00 41.01
ATOM	3206	C	ALA		515 515	61.767	5.018	30.444	1.00 42.33
ATOM	3207	0	ALA		515	64.099	5.683	31.147	1.00 40.47
ATOM	3208	N	SER		516	64.291	6.690	31.831	1.00 41.28
ATOM	3209	CA	SER		516	64.788	4.553	31.307	1.00 38.78
MOTA	3210	СВ	SER		16	65.806	4.441	32.347	1.00 40.97
ATOM	3211	OG	SER		16	66.354	3.009	32.454	1.00 37.82
ATOM	3212	C	SER		16	67.172	2.651	31.359	1.00 34.73
ATOM	3213	0	SER		16	66.941	5.416	32.061	1.00 42.68
ATOM	3214	N	LYS		17	67.714	5.769	32.957	1.00 45.78
ATOM	3215	CA	LYS		17 17	67.015	5.869	30.815	1.00 40.92
ATOM	3216	CB	LYS		17	68.025	6.816	30.380	1.00 38.04
ATOM	3217	CG	LYS		17	68.541	6.411	29.003	1.00 38.25
MOTA	3218	CD	LYS		17	69.293	5.111	29.021	1.00 36.40
				٠,	- 1	70.421	5.221	29.992	1.00 38.14



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MOTA	3219	CE	LYS	617	71.215	3.941	30.086	1.00	38.43
MOTA	3220	NZ	LYS	617	72.530	4.210	30.751	1.00	43.07
ATOM	3221	С	LYS	617	67.475	8.242	30.350	1.00	38.42
ATOM	3222	0	LYS	617	68.072	9.133	29.744	1.00	41.37
ATOM	3223	N	LYS	618	66.323	8.444	30.985	1.00	37.25
ATOM	3224	CA	LYS	618	65.674	9.743	31.067	1.00	36.75
ATOM	3225	CB	LYS	618	66.653	10.780	31.632	1.00	43.27
MOTA	3226	CG	LYS	618	67.340	10.392	32.938	1.00	51.59
MOTA	3227	CD	LYS	618	66.377	10.361	34.092	1.00	61.24
ATOM	3228	CE	LYS	618	67.070	9.945	35.373	1.00	67.83
MOTA	3229	NZ	LYS	618	66.105	10.039	36.510	1.00	75.22
MOTA	3230	С	LYS	618	65.167	10.222	29.706	1.00	36.61
ATOM	3231	0	LYS	618	64.856	11.396	29.535	1.00	35.94
ATOM	3232	N	CYS	619	65.058	9.308	28.751		36.26
ATOM	3233	CA	CYS	619	64.603	9.666	27.412		33.41
ATOM	3234	CB	CYS	619	65.351	8.843	26.365		32.17
ATOM	3235	SG	CYS	619	65.006	9.223	24.650		26.92
MOTA	3236	С	CYS	619	63.108	9.546	27.194		32.29
ATOM	3237	0	CYS	619	62.510	8.472	27.373	1.00	29.13
ATOM	3238	N	ILE	620	62.515	10.679	26.827	1.00	31.60
ATOM	3239	CA	ILE	620	61.091	10.763	26.528	1.00	31.21
ATOM	3240	CB	ILE	620	60.435	11.966	27.212	1.00	29.57
ATOM	3241	CG2	ILE	620	58.955	12.031	26.860	1.00	31.49
MOTA	3242	CG1	ILE	620	60.578	11.848	28.727	1.00	27.85
ATOM	3243	CD1	ILE	620	60.065	13.046	29.463	1.00	26.50
MOTA	3244	С	ILE	620	61.034	10.972	25.018	1.00	32.18
MOTA	3245	0	ILE	620	61.481	11.993	24.512	1.00	33.18
MOTA	3246	N	HIS	621	60.472	9.990	24.318	1.00	31.93
MOTA	3247	CA	HIS	621	60.354	9.970	22.864	1.00	32.59
MOTA	3248	CB	HIS	621	59.933	8.552	22.420	1.00	29.51
MOTA	3249	CG	HIS	621	60.076	8.288	20.951	1.00	27.45
MOTA	3250	CD2	HIS	621	60.663	7.262	20.286	1.00	25.84
MOTA	3251	ND1	HIS	621	59.528	9.106	19.979	1.00	25.20
ATOM	3252	CE1	HIS	621	59.774	8.596	18.783	1.00	25.07
MOTA	3253	NE2	HIS	621	60.456	7.473	18.942	1.00	23.24
ATOM	3254	C	HIS	621	59.365	10.992	22.320	1.00	35.31
MOTA	3255	0	HIS	621	59.555	11.481	21.220		39.24
ATOM	3256	N	ARG	622	58.256	11.216	23.028	1.00	36.50
MOTA	3257	CA	ARG	622	57.225	12.169	22.580	1.00	35.78
MOTA	3258	CB	ARG	622	57.783	13.582	22.462		32.55
MOTA	3259	CG	ARG	622	58.211	14.156	23.778	1.00	30.54
MOTA	3260	CD	ARG	622	58.799	15.551	23.635	0.50	
ATOM	3261	NE	ARG	622	59.249	16.043	24.930	0.50	24.53
MOTA	3262	CZ	ARG	622	60.409	15.707	25.499	0.50	
ATOM	3263		ARG	622	61.249	14.883	24.877	0.50	
ATOM	3264		ARG	622	60.711	16.158	26.714	0.50	
ATOM	3265	С	ARG	622	56.447	11.806	21.297	1.00	
ATOM	3266	0	ARG	622	55.438	12.430	20.999	1.00	36.61
ATOM	3267	N	ASP	623	56.923	10.818	20.537	1.00	
MOTA	3268	CA	ASP	623	56.197	10.400	19.335	1.00	
MOTA	3269	CB	ASP	623	56.628	11.171	18.081	1.00	34.77
ATOM	3270	CG	ASP	623	55.727	10.869	16.863	1.00	43.51



ATO	M 32	77 /	201 701					
ATO			OD1 ASI		56.21	3 10.99	2 15.714	1.00 47.45
ATO			DD2 ASI		54.53		9 17.032	
ATO					56.32	1 8.903		
ATO			ASI		56.63	5 8.435		
ATO			LEU		56.08	1 8.135		
			A LEU		56.15	2 <b>6.68</b> 9		
ATON			B LEU		56.13			
MOTA			G LEU		55.98			
ATOM			DI LEU		57.108			
ATOM		0 C	D2 LEU	624	56.00			1.00 23.96
ATOM			LEU	624	54.954	-	19.187	1.00 29.50
ATOM			LEU	624	53.805		19.505	1.00 32.04
ATOM	_		ALA	625	55.224			1.00 36.02
ATOM		4 C	A ALA	625	54.170		18.076	1.00 28.91
ATOM		5 C	B ALA	625	53.707		17.192	1.00 25.66
ATOM		e C	ALA	625	54.800		16.289	1.00 23.37
ATOM		7 0	ALA	625	56.022		16.389	1.00 27.71
ATOM	328	в и	ALA	626	53.982		16.355	1.00 29.77
MOTA	3289	9 C		626	54.499		15.758	1.00 29.46
ATOM	3290	) CE	ALA	626	53.350		14.956	1.00 28.16
ATOM	3291	L C	ALA	626	55.366		14.401	1.00 28.02
ATOM	3292	2 0	ALA	626	56.329	2.504	13.831	1.00 26.78
ATOM	3293	N	ARG	627	55.022	1.859	13.454	1.00 26.69
ATOM	3294	CA		627		3.680	13.314	1.00 26.09
ATOM	3295	CB		627	55.777	4.301	12.246	1.00 26.78
ATOM	3296			627	55.134	5.637	11.837	1.00 27.01
ATOM	3297			627	55.046	6.672	12.961	1.00 29.34
ATOM	3298		ARG	627	54.552	8.037	12.477	1.00 34.26
ATOM	3299		ARG	627	54.108	8.878	13.590	1.00 36.96
ATOM	3300		1 ARG	627	52.867	8.889	14.059	1.00 40.84
ATOM	3301		2 ARG	627	51.942	8.114	13.515	1.00 42.56
ATOM	3302	C	ARG	627	52.552	9.634	15.108	1.00 45.20
ATOM	3303	ō	ARG		57.209	4.549	12.711	1.00 29.11
ATOM	3304	N		627	58.137	4.468	11.911	1.00 30.39
ATOM	3305	CA	ASN	628	57.385	4.804	14.010	1.00 30.37
ATOM	3306	CB	ASN	628	58.689	5.092	14.596	1.00 27.02
ATOM	3307	CG	ASN	628	58.578	6.226	15.611	1.00 24.35
ATOM	3308		ASN ASN	628	58.383	7.571		1.00 25.95
ATOM	3309		ASN	628	58.992	7.865		1.00 32.01
ATOM	3310	C		628	57.522			1.00 24.34
ATOM	3311	0	ASN	628	59.437	3.903	15.185	1.00 26.74
ATOM	3312		ASN	628	60.378			1.00 28.49
ATOM		N	VAL	629	58.998			1.00 27.34
ATOM	3313	CA	VAL	629	59.621			1.00 24.94
ATOM	3314	CB	VAL	629	58.589			1.00 22.20
	3315		VAL	629	59.169			
ATOM ATOM	3316		VAL	629	58.158			1.00 18.03 1.00 18.34
	3317	C .	VAL	629	60.077			L.00 26.84
ATOM	3318	0	VAL	629	59.284			
ATOM	3319	N	LEU	630	61.352			26.50
ATOM	3320	CA	LEU	630	61.862	_		27.66
ATOM	3321	CB	LEU	630	63.105			.00 30.14
MOTA	3322	CG	LEU	630	62.856			.00 28.00
							L2.027 1	.00 26.06



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ATOM	3323	CD1	LEU	630	64.150	2.831	11.832	1.00	23.44
MOTA	3324	CD2	LEU	630	61.880	2.381	10.901	1.00	27.72
ATOM	3325	С	LEU	630	62.145	-1.627	12.889	1.00	32.90
ATOM	3326	0	LEU	630	62.437	-1.982	14.029	1.00	33.06
MOTA	3327	N	VAL	631	61.991	-2.478	11.873	1.00	34.83
ATOM	3328	CA	VAL	631	62.195	-3.928	12.006	1.00	33.02
ATOM	3329	CB	VAL	631	60.915	-4.700	11.584	1.00	30.92
MOTA	3330	CG1	VAL	631	61.071	-6.208	11.842	1.00	27.66
ATOM	3331	CG2	VAL	631	59.724	-4.161	12.332	1.00	24.46
ATOM	3332	С	VAL	631	63.371	-4.415	11.161	1.00	35.77
ATOM	3333	0	VAL	631	63.428	-4.171	9.954	1.00	37.57
ATOM	3334	N	THR	632	64.319	-5.098	11.797	1.00	37.96
MOTA	3335	CA	THR	632	65.511	-5.599	11.096	1.00	39.06
MOTA	3336	CB	THR	632	66.675	-5.820	12.066	1.00	35.55
MOTA	3337	OG1	THR	632	66.368	-6.903	12.955	1.00	35.76
ATOM	3338	CG2	THR	632	66.928	-4.561	12.867	1.00	35.06
ATOM	3339	C	THR	632	65.283	-6.893	10.331	1.00	40.66
ATOM	3340	0	THR	632	64.238	-7.515	10.466	1.00	41.79
MOTA	3341	N	GLU	633	66.282	-7.307	9.556	1.00	43.40
MOTA	3342	CA	GLU	633	66.219	-8.540	8.768	1.00	45.33
ATOM	3343	CB	GLU	633	67.501	-8.689	7.942	1.00	48.67
ATOM	3344	CG	GLU	633	67.496	-9.791	6.864	1.00	54.70
ATOM	3345	CD	GLU	633	66.599	-9.506	5.647		58.16
ATOM	3346	OE1	GLU	633	<b>65.93</b> 3	-8.452	5.567	1.00	60.68
ATOM	3347	OE2	GLU	633	66.566	-10.369	4.747	1.00	60.14
ATOM	3348	C	GLU	633 .	66.011	-9.774	9.648	1.00	46.02
MOTA	3349	0	GLU	633	65.637	-10.834	9.156	1.00	46.75
MOTA	3350	N	ASP	634	66.278	-9.648	10.944	1.90	46.45
ATOM	3351	CA	ASP	634	65.085	-10.774	11.843	1.00	46.14
ATOM	3352	CB	ASP	634	67.316	-10.995	12.724	1.00	52.89
ATOM	3353	CG	ASP	634	68.570	-11.399	11.929	1.00	59.65
MOTA	3354		ASP	634	68.593	-12.499	11.328		59.91
ATOM	3355		ASP	634	69.546	-10.608	11.918	1.00	62.29
MOTA	3356	C	ASP	634	64.850	-10.549	12.708	1.00	45.75
MOTA	3357	0	ASP	634	64.729	-11.138	13.776	1.00	46.38
ATOM	3358	N	ASN	635	63.940	-9.697	12.235	1.00	45.92
ATOM	3359	CA	ASN	635	62.690	-9.367	12.915	1.00	44.36
ATOM	3360	CB	ASN	635	61.750	-10.583	12.972	1.00	46.62
ATOM	3361	CG	ASN	635		-11.116	11.597	1.00	47.56
MOTA	3362	OD1		635		-10.453	10.800	1.00	
ATOM	3363	ND2		635		-12.314	11.305	1.00	47.75
ATOM	3364	С	ASN	635	62.833	-8.763	14.308	1.00	
ATOM	3365	0	ASN	635	62.028	-9.045	15.189	1.00	
MOTA	3366	N	VAL	636	63.849	-7.927	14.503	1.00	
ATOM	3367	CA	VAL	636	64.071	-7.291	15.797	1.00	36.87
ATOM	3368	CB	VAL	636	65.584	-7.162	16.083	1.00	
ATOM	3369	CG1		636	65.839	-6.347	17.354	1.00	
ATOM	3370	CG2		636	66.184	-8.535	16.226	1.00	
ATOM	3371	С	VAL	636	63.434	-5.908	15.782	1.00	
ATOM	3372	0	VAL	636	63.657	-5.131	14.854	1.00	36.58
ATOM	3373	N	MET	637	62.600	-5.625	16.773	1.00	32.04
MOTA	3374	CA	MET	637	61.940	-4.331	16.887	1.00	31.14



ATC		375	CB M	ET 637	60.7	34 -4 4	22 4	_
ATO		176	CG M	ET 637	59.7			
ATO		77	SD M	ET 637	58.8			
ATO			CE M	ET 637	59.1		5	02
ATO.			C MI	ET 637	62.9	· · ·	_ =	
ATO			M C	ET 637	63.5			
ATO			7 L	'S 638	63.04			
ATO		82 (	CA LY		63.9			
ATO		83 (	B LY		65.21			01
ATON		84 (	G LY		66.14			
ATON		35 (	D LY		67.30			
ATOM			E LY	S 638	68.36			
ATOM		37 N	Z LY		68.93			
ATOM		-	LY	S 638	63.36	_	_	
ATOM		_	LY	S 638	62.98			
ATOM		0 N	IL		63.27			
ATOM			A ILI	E 639	62.73			
ATOM	339	2 C	B IL	E 639	62.69	_		
ATOM	339	3 C	32 ILE	639	61.91	_		1.00 23.98
ATOM	339	-	31 ILE		62.12			1.00 21.11
ATOM	339		Ol ILE	639	60.680			1.00 26.06
ATOM	339	-	ILE	639	63.656			1.00 28.45
MOTA	339		ILE	639	64.884			1.00 26.36
ATOM	3398		ALA	640	63.073	_		1.00 25.06
ATOM	3399		ALA	640	63.857			1.00 26.70
ATOM	3400		ALA	640	63.683			1.00 27.85
ATOM	3401	_	ALA	640	63.380			1.00 27.66
ATOM	3402	_	ALA	640	62.307		16.548	1.00 29.56
ATOM	3403		ASP	641	64.174		17.136	1.00 29.82
, ATOM	3404		ASP	641	63.863	8.874	16.180	1.00.28.74
ATOM	3405		ASP	641	62.662	9.310	16.415	1.00 32.13
ATOM	3406	CG	ASP	641	63.024	9.555		1.00 35.25
ATOM	3407		l Asp	641	64.149	9.170	14.121	1.00 38.54
ATOM	3408		ASP	641	62.192	10.144	13.716	1.00 39.85
ATOM	3409	C	ASP	641	63.661	9.311	13.394	1.00 41.38
ATOM	3410	0	ASP	641	63.012	10.323	17.862	1.00 30.61
ATOM ATOM	3411	N	PHE	642	64.265	8.567	18.140 18.776	1.00 29.45
ATOM	3412	CA	PHE	642	64.155	8.860	20.195	1.00 30.96
ATOM	3413	CB	PHE	642	64.447	7.597		1.00 31.21
ATOM	3414	CG	PHE	642	65.806	7.008		1.00 27.06
ATOM	3415		PHE	642	66.930	7.476		1.00 24.27
	3416		PHE	642	65.962	5.978		1.00 22.36
ATOM	3417		PHE	642	68.179	6.928		1.00 24.87
ATOM ATOM	3418	CE2		642	67.205	5.420		1.00 23.19
	3419	CZ	PHE	642	68.323	5.898		1.00 23.65
ATOM	3420	C	PHE	642	65.069	10.007		1.00 22.95
ATOM	3421	0	PHE	642	64.920	10.549		1.00 34.88
ATOM	3422	N	GLY	643	66.000	10.377	21.729 ; 19.737 ;	1.00 34.84
ATOM	3423	CA	GLY	643	66.934	11.450		1.00 36.20
ATOM	3424	C .	GLY	643	66.728	12.720	-	1.00 35.47
ATOM	3425	0	GLY	643	67.581	13.593	19.232	00 37.62
ATOM	3426	N	LEU	644	65.609		19.269 1	00 39.16
						,	18.517 1	.00 39.68



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ATOM	3427	CA	LEU	644	65.328	14.029	17.712	1.00 43.09
ATOM	3428	CB	LEU	644	64.074	13.843	16.860	1.00 40.78
MOTA	3429	CG	LEU	644	64.076	12.876	15.681	1.00 36.94
ATOM	3430		LEU	644	62.790	13.076	14.901	1.00 37.34
MOTA	3431		LEU	644	65.240	13.157	14.783	1.00 37.72
ATOM	3432	C	LEU	644	65.154	15.261	18.591	1.00 47.32
ATOM	3433	0	LEU	644	64.639	15.170	19.702	1.00 50.33
MOTA	3434	N	ALA	645	65.598	16.406	18.088	1.00 51.23
MOTA	3435	CA	ALA	645	65.507	17.662	18.820	1.00 52.97
ATOM	3436	CB	ALA	645	66.367	18.703	18.151	1.00 54.12
ATOM	3437	С	ALA	645	64.060	18.137	18.910	1.00 53.00
MOTA	3438	0	ALA	645	63.591	18.528	19.977	1.00 53.59
MOTA	3439	N	ASP	652	52.356	21.675	14.855	1.00 79.51
MOTA	3440	CA	ASP	652	51.194	21.821	13.993	1.00 78.74
MOTA	3441	CB	ASP	652	51.625	22.021.	12.531	1.00 78.30
MOTA	3442	CG	ASP	652	50.459	22.358	11.608	1.00 77.64
MOTA	3443	OD1		652	49.473	22.968	12.079	1.00 77.67
ATOM	3444	OD2	ASP	652	50.526	22.029	10.410	1.00 78.25
ATOM	3445	С	ASP	652	50.339	20.569	14.125	1.00 78.92
ATOM	3446	0	ASP	652	50.645	19.529	13.539	1.00 79.36
MOTA	3447	N	TYR	653	49.262	20.682	14.892	1.00 79.17
MOTA	3448	CA	TYR	653	48.357	19.560	15.111	1.00 80.23
ATOM	3449	CB	TYR	653	47.283	19.932	16.136	1.00 81.36
MOTA	3450	CG	TYR	653	47.790	20.060	17.557	1.00 84.51
ATOM	3451	CD1		653	46.998	20.649	18.544	1.00 86.09
ATOM	3452	CE1	TYR	653	47.443	20.751	19.865	1.00 88.05
ATOM	3453	CD2	TYR	653	49.049	19.576	17.925	1.00 86.22
ATOM	3454	CE2	TYR	653	49.504	19.673	19.242	1.00 87.14
ATOM	3455	CZ	TYR	653	48.698	20.260	20.207	1.00 88.37
ATOM	3456	OH	TYR	653	49.146	20.351	21.510	1.00 88.82
ATOM	3457	C	TYR	653	47.687	19.098	13.827	1.00 80.07
ATOM	3458	0	TYR	653	47.170	17.983	13.752	1.00 81.23
ATOM	3459	N	TYR	654	47.716	19.953	12.813	1.00 79.01
ATOM	3460	CA	TYR	654	47.082	19.640	11.544	1.00 78.81
ATOM	3461	CB	TYR	654	46.378	20.884	11.008	1.00 78.48
ATOM	3462	CG	TYR	654	45.358	21.422	11.982	1.00 78.53
ATOM	3463	CD1		654	45.752	21.948	13.213	1.00 77.46
ATOM	3464	CE1		654	44.822	22.382	14.146	1.00 78.94
ATOM	3465	CD2		654	43.997	21.350	11.704	1.00 80.18
ATOM	3466		TYR	654	43.054	21.785	12.632	1.00 82.55
ATOM	3467	CZ	TYR	654	43.473	22.295	13.851	1.00 80.98
MOTA	3468	OH	TYR	654	42.548	22.703	14.785	1.00 82.29
ATOM	3469	C	TYR	654	48.010	19.042	10.499	1.00 79.04
ATOM	3470	0	TYR	654	47.575	18.720	9.393	1.00 80.09
ATOM	3471	N	LYS	655	49.277	18.859	10.848	1.00 78.74
ATOM	3472	CA	LYS	655	50.217	18.282	9.906	1.00 80.69
ATOM	3473	CB	LYS	655	51.651	18.687	10.247	1.00 83.97
ATOM	3474	CG	LYS	655	52.674	18.124	9.281	1.00 89.76
ATOM	3475	CD	LYS	655	54.084	18.565	9.611	1.00 93.90
ATOM	3476	CE	LYS	655	55.075	17.844	8.708	1.00 97.62
MOTA	3477	NZ	LYS	655	56.489	18.177	9.038	1.00101.35
ATOM	3478	С	LYS	655	50.070	16.763	9.922	1.00 80.98

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ATOM	3496				47.900	8.861		1.00 48.40
ATOM	3497			661	47.612	7.566		1.00 49.76
ATOM	3498			661	47.80]	6.331		1.00 52.48
ATOM	3499			661	47.691		9.734	1.00 52.60
ATOM	3500			661	47.955		10.264	1.00 50.93
ATOM	3501		1 ARG	661	48.343		11.529	1.00 48.54
ATOM	3502		2 ARG	661	47.836		9.523	1.00 52.75
ATOM	3502	_	ARG	661	47.894		10.439	1.00 43.81
ATOM	3504	_	ARG	661	48.833		10.063	1.00 43.23
ATOM	3505		LEU	662	47.194	11.618	11.537	1.00 40.56
ATOM	3506	CB		662	47.496	12.735	12.428	1.00 37.52
ATOM	3507	CG	LEU	662	46.220	13.496	12.789	1.00 33.26
ATOM	3508		LEU 1 LEU	662	45.485	14.281	11.696	1.00 31.29
ATOM	3509		2 LEU	662	44.084	14.621	12.158	1.00 24.03
ATOM	3510	C C	LEU	662	46.261	15.535	11.358	1.00 28.65
ATOM	3511	o	LEU	662	48.154	12.237	13.712	1.00 36.78
ATOM	3512	N	PRO	662 663	47.515	11.570	14.536	1.00 37.27
ATOM	3513	CD	PRO	663 663	49.448	12.549	13.895	1.00 36.46
ATOM	3514	CA	PRO	663	50.320	13.216	12.914	1.00 38.35
ATOM	3515	СВ	PRO	663 663	50.224	12.148		1.00 35.98
ATOM	3516	CG	PRO	663	51.537	12.887	14.872	1.00 34.95
ATOM	3517	C	PRO	663	51.702	12.836		1.00 39.18
ATOM	3518	ō	PRO	663	49.569	12.499		1.00 35.53
ATOM	3519	N	VAL	664	49.779	11.814	17.399	1.00 38.34
ATOM	3520	CA	VAL	664	48.759	13.558	16.414	1.00 32.71
ATOM	3521	CB	VAL	664	48.080	13.964	17.632	1.00 30.18
ATOM	3522		VAL	664	47.195	15.242	17.427	1.00 31.31
MOTA	3523		VAL	664	48.060	16.409	17.038	L.00 28.93
ATOM	3524	C	VAL	664	46.143	15.038	16.345	1.00 34.42
ATOM	3525	Ō	VAL	664	47.268	12.787	18.172	00 29.48
ATOM	3526	N	LYS	665	47.080		19.388 1	.00 30.41
ATOM	3527	CA	LYS	665	46.873		17.282 1	.00 29.29
ATOM	3528	СВ	LYS .	665	46.105		17.668 1	.00 28.55
ATOM	3529	CG	LYS	665	45.517		16.423 1	.00 26.97
ATOM	3530	CD	LYS	665	44.415		15. <b>78</b> 6 1	.00 27.88
				~ <del></del>	43.979	10.366	14.418 1	.00 29.41

ATOM	3531	CE	LYS	665	42.785	11.162	13.899	1.00 26.35
MOTA	3532	NZ	LYS	665	42.363	10.809	12.508	1.00 26.16
ATOM	3533	С	LYS	665	46.890	9.730	18.556	1.00 28.81
MOTA	3534	0	LYS	665	46.315	8.802	19.113	1.00 29.38
MOTA	3535	N	TRP	666	48.181	9.976	18.736	1.00 28.98
ATOM	3536	CA	TRP	666	49.005	9.128	19.599	1.00 31.67
ATOM	3537	CB	TRP	666	50.323	8.755	18.913	1.00 29.46
ATOM	3538	CG	TRP	666	50.205	7.582	17.977	1.00 28.92
MOTA	3539	CD2	TRP	666	49.676	7.603	16.642	1.00 27.62
ATOM	3540	CE2	TRP	666	49.740	6.276	16.162	1.00 27.15
ATOM	3541	CE3	TRP	666	49.151	8.607	15.818	1.00 25.27
ATOM	3542	CD1	TRP	666	50.565	6.289	18.238	1.00 24.30
ATOM	3543	NE1	TRP	666	50.287	5.506	17.147	1.00 27.82
ATOM	3544	CZ2	TRP	666	49.295	5.930	14.872	1.00 26.95
ATOM	3545	CZ3	TRP	666	48.707	8.256	14.536	1.00 25.95
ATOM	3546	CH2	TRP	666	48.778	6.929	14.081	1.00 28.35
ATOM	3547	C	TRP	666	49.316	9.836	20.907	1.00 33.46
ATOM	3548	0	TRP	<b>6</b> 66	49.790	9.219	21.867	1.00 34.77
ATOM	3549	N	MET	667	49.021	11.128	20.947	1.00 35.61
ATOM	3550	CA	MET	667	49.306	11.948	22.110	1.00 37.94
ATOM	3551	CB	MET	667	49.308	13.419	21.723	1.00 40.22
ATOM	3552	CG	MET	667	50.606	13.939	21.150	1.00 40.77
ATOM	3553	SD	MET	667	50.479	15.723	20.906	1.00 44.04
MOTA	3554	CE	MET	667	50.932	15.858	19.204	1.00 39.07
ATOM	3555	C	MET	667	48.432	11.775	23.346	1.00 39.61
ATOM	3556	0	MET	667	47.211	11.672	23.255	1.00 42.46
ATOM	3557	N	ALA	668	49.072	11.820	24.505	1.00 38.46
ATOM	3558	CA	ALA	668	48.383	11.704	25.773	1.00 37.78
ATOM	3559	CB	ALA	668	49.388	11.473	26.894	1.00 38.21
ATOM	3560	C	ALA	668	47.666	13.033	25.966	1.00 37.46
ATOM ATOM	3561	N O	ALA	668	48.156	14.072	25.521	1.00 35.74
ATOM	3562 3563	CD	PRO PRO	669 669	46.521	13.027	26.665 27.243	1.00 37.55
ATOM	3564	CA	PRO	669	45.868	11.840 14.229		1.00 38.19
ATOM	3565	CB			45.723		26.923	1.00 39.30
ATOM	3566	CG	PRO PRO	669 669	44.638	13.708 12.301	27.864 27.379	1.00 39.82 1.00 39.13
ATOM	3567	C	PRO	669	44.444 46.517	15.391	27.535	1.00 39.13
ATOM	3568	0	PRO	669	46.442	16.523	27.056	1.00 40.33
ATOM	3569	N	GLU	670	47.303	15.113	28.569	1.00 41.15
ATOM	3570	CA	GLU	670	48.096	16.169	29.200	1.00 42.80
ATOM	3571	СВ	GLU	670	48.776	15.657	30.464	1.00 42.97
ATOM	3572	CG	GLU	670	49.928	14.705	30.205	1.00 42.82
ATOM	3573	CD	GLU	670	49.506	13.252	30.150	1.00 44.16
ATOM	3574	OE1	GLU	670	50.395	12.384	30.257	1.00 40.43
ATOM	3575	OE2	GLU	670	48.297	12.974	30.013	1.00 46.36
ATOM	3576	C	GLU	670	49.145	16.795	28.276	1.00 43.00
ATOM	3577	0	GLU	670	49.435	17.979	28.380	1.00 40.37
ATOM	3578	N	ALA	671	49.697	15.999	27.367	1.00 44.03
ATOM	3579	CA	ALA	671	50.708	16.495	26.440	1.00 44.90
ATOM	3580	CB	ALA	671	51.460	15.333	25.814	1.00 42.47
ATOM	3581	C	ALA	671	50.063	17.364	25.361	1.00 47.79
ATOM	3582	ō	ALA	671	50.602	18.398	24.977	1.00 47.27
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ATOM	3587		1 LEU	672	47.23			57.15
ATOM	3588		2 LEU	672	45.44			
MOTA	3589	_	LEU	672	47.456			
ATOM	3590	_	LEU	672	47.502			
MOTA	3591		PHE	673	46.866			
MOTA	3592		PHE	673	46.179			
ATOM	3593		PHE	673	44.974			
ATOM	3594		PHE	673	43.967		26.200	
ATOM	3595		l PHE	673	43.477		26.580	
ATOM	3596		2 PHE	673	43.491		25.022	
ATOM	3597		PHE	673	42.530		25.808	1.00 53.89
ATOM	3598		PHE	673	42.540		24.239	1.00 55.44
ATOM	3599	CZ	PHE	673	42.062		24.637	1.00 54.80 1.00 54.86
ATOM	3600	С	PHE	673	47.071		27.200	1.00 54.86
ATOM	3601	0	PHE	673	47.084	21.959	27.095	
ATOM	3602	N	ASP	674	47.832	20.086	28.077	1.00 60.79
ATOM	3603	CA	ASP	674	48.698	20.798	29.026	1.00 60.63 1.00 61.52
ATOM	3604	CB	ASP	674	48.638	20.137	30.410	1.00 61.32
ATOM	3605	CG	ASP	674	47.247	20.143	31.010	
ATOM	3606		ASP	674	46.706	19.039	31.246	1.00 62.87 1.00 62.99
ATOM	3607		ASP	674	46.698	21.239	31.253	1.00 63.55
ATOM	3608	С	ASP	674	50.176	20.898	28.618	1.00 61.58
ATOM	3609	0	ASP	674	51.014	21.284	29.446	1.00 60.41
ATOM	3610	N	ARG	675	50.499	20.519	27.380	1.00 61.38
ATOM	3611	CA	ARG	675	51.885	20.526	26.883	1.00 59.23
ATOM	3612	CB	ARG	675	52.336	21.944	26.515	1.00 59.05
ATOM	3613	CG	ARG	675	51.548	22.564	25.367	1.00 64.48
ATOM	3614	CD	ARG	675	52.036	23.967	25.014	1.00 68.61
ATOM	3615	NE	ARG	675	53.348	23.969	24.359	1.00 69.16
ATOM	3616	CZ	ARG	675	54.076	25.061	24.145	1.00 68.19
ATOM	3617	NH1		675	53.622	26.250	24.531	1.00 66.97
ATOM	3618	NH2		675	55.265	24.965	23.564	1.00 67.00
ATOM	3619	C	ARG	675	52.849	19.885	27.892	1.00 57.27
ATOM	3620		ARG	675	54.002	20.300	28.033	1.00 57.05
ATOM	3621	N	ILE	676	52.356	18.867	28.591	1.00 57.05
ATOM	3622		ILE	676	53.136	18.140	29.589	1.00 53.44
ATOM	3623		ILE	676	52.314	17.899	30.874	1.00 50.96
ATOM	3624		ILE	676	52.934	16.787	31.718	1.00 47.57
ATOM	3625		ILE	676	52.213	19.196	31.669	1.00 47.57
ATOM	3626	CD1	ILE	676	51.443	19.073	32 964	1.00 50.88

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**ATOM** 3635 CD2 TYR 677 55.140 15.251 24.829 1.00 56.63 ATOM 3636 CE2 TYR 677 54.459 15.654 23.680 1.00 54.84 **ATOM** 3637 CZTYR 23.490 1.00 56.38 677 54.183 17.004 **ATOM** 3638 OH TYR 677 53.555 17.426 22.340 1.00 57.46 **ATOM** 3639 C TYR 677 56.268 14.713 29.304 1.00 51.49 MOTA 3640 0 TYR 677 57.186 15.283 29.904 1.00 52.65 MOTA 29.579 3641 N THR 678 55.881 13.471 1.00 48.54 MOTA 3642 CA THR 678 56.571 12.648 30.568 1.00 46.14 MOTA 3643 CB THR 678 55.776 12.597 31.910 1.00 47.34 MOTA OG1 THR 3644 678 54.615 11.764 31.764 1.00 50.96 MOTA 3645 CG2 THR 678 55.346 13.996 32.345 1.00 47.47 MOTA 3646 С THR 678 56.742 11.218 30.041 1.00 43.21 MOTA 3647 THR 678 0 56.371 10.917 28.912 1.00 41.64 MOTA 3648 N HIS 679 57.334 10.351 30.854 1.00 42.21 **ATOM** 3649 CA HIS 679 57.507 8.969 30.456 1.00 39.96 ATOM 3650 CB HIS 679 58.410 8.216 31.428 1.00 39.23 **ATOM** 3651 CG HIS 679 59.833 8.677 31.418 1.00 43.24 **ATOM** 3652 CD2 HIS 679 60.501 9.505 32.253 1.00 43.12 **ATOM** 3653 ND1 HIS 679 60.759 8.236 30.498 1.00 42.63 **ATOM** 3654 CE1 HIS 679 61.938 8.762 30.774 1.00 42.66 MOTA 3655 NE2 HIS 679 61.807 9.539 31.832 1.00 43.80 MOTA 3656 С HIS 679 56.145 8.301 30.429 1.00 40.78 **ATOM** 3657 0 HIS 679 55.930 7.358 29.678 1.00 42.66 ATOM 3658 N GLN 680 55.227 8.803 31.254 1.00 40.26 ATOM 3659 CA GLN 680 53.881 8.261 1.00 39.10 31.324 ATOM 3660 GLN CB 680 53.187 8.664 32.625 1.00 39.23 ATOM 3661 CG GLN 680 53.762 7.980 33.874 1.00 41.07 **ATOM** 3662 CD GLN 680 53.813 6.450 33.770 1.00 39.96 **ATOM** 3663 OE1 GLN 680 52.818 5.762 33.993 1.00 39.53 ATOM 3664 NE2 GLN 54.990 680 5.919 33.464 1.00 32.85 ATOM 3665 C GLN 680 53.070 8.676 30.103 1.00 39.20 ATOM 3666 0 GLN 680 52.194 7.933 1.00 39.29 29.656 **ATOM** 3667 N SER 681 53.368 9.843 29.531 1.00 38.01 **ATOM** 3668 CA SER 681 52.656 10.264 28.325 1.00 39.27 MOTA 3669 CB SER 681 52.979 11.712 27.968 1.00 40.93 MOTA 3670 OG SER 681 54.366 11.936 27.943 1.00 39.70 MOTA 3671 C 1.00 39.93 SER 681 53.090 9.309 27.208 ATOM 3672 0 SER 681 52.285 8.953 26.335 1.00 40.46 **ATOM** 3673 N ASP 682 54.356 8.881 27.269 1.00 37.28 **ATOM** 3674 ASP CA 682 54.920 7.921 26.315 1.00 35.38 ATOM 3675 CB ASP 682 56.411 7.673 26.586 1.00 33.58 MOTA 3676 CG ASP 682 57.332 8.520 25.717 1.00 33.16 MOTA 3677 OD1 ASP 682 58.545 8.283 25.828 1.00 31.76 ATOM 3678 OD2 ASP 682 56.886 9.391 24.936 1.00 30.06 MOTA 3679 C ASP 682 54.178 6.599 26.463 1.00 34.70 **ATOM** 3680 ASP 0 682 54.012 5.868 25.488 1.00 35.67 MOTA 3681 N VAL 683 53.758 6.296 27.691 1.00 34.44 MOTA 3682 CA VAL 683 53.011 5.072 27.987 1.00 35.14 **ATOM** 3683 CB VAL 683 52.895 4.852 29.544 1.00 35.48 MOTA 3684 CG1 VAL 683 51.752 3.900 29.890 1.00 34.95 **ATOM** 3685 CG2 VAL 683 54.202 4.282 30.080 1.00 28.77 ATOM 3686 C VAL 683 51.638 5.091 27.279 1.00 32.81

ATOM		7 0	VAI	683	51.17	73 4.05	0 25 22	
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ATOM	369	2 CD	2 TRP		46.63			
ATOM	369	3 CE	2 TRP		45.85			· <b></b>
ATOM	3694	4 CE	3 TRP	684	46.02			
ATOM	3699	5 CD		684	47.93			
ATOM	3696	5 NE		684	46.66			
ATOM	3697	7 CZ		684	44.48			
ATOM	3698	cz cz		684				
MOTA	36.99	CH:		684	44.668 43.918			
ATOM	3700		TRP	684	49.94			
ATOM	3701	. 0	TRP	684				
ATOM	3702	N	SER	685	49.214			1.00 32.25
ATOM	3703	CA	SER	685	50.977			1.00 28.90
ATOM	3704	СВ	SER	685	51.345			1.00 27.10
ATOM	3705		SER	685	52.620			1.00 23.88
ATOM	3706	C	SER	685	52.459			1.00 25.82
ATOM	3707	0	SER	685	51.567		22.786	1.00 27.85
MOTA	3708	N	PHE	686	51.172		21.746	1.00 28.89
ATOM	3709	CA	PHE	686	52.178		23.741	1.00 28.84
ATOM	3710	CB	PHE	686	52.410		23.622	1.00 27.86
ATOM	3711	CG	PHE	686	53.255		24.800	1.00 28.14
ATOM	3712		PHE	686	53.498		24.803	1.00 28.41
ATOM	3713	CD2		686	54.256	0.313	23.802	1.00 27.54
ATOM	3714		PHE	686	52.949	0.109	25.796	1.00 29.15
ATOM	3715	CE2		686	54.465	-1.057	23.792	1.00 24.25
MOTA	3716	CZ	PHE	686	53.151	-1.268	25.7 <b>9</b> 0	1.00 27.86
MOTA	3717	C	PHE	686	53.912	-1.850	24.782	1.00 26.09
ATOM	3718	0	PHE	686	51.072	2.122	23.566	1.00 30.99
MOTA	3719	N	GLY	687	50.960	1.109	22.873	1.00 29.21
ATOM	3720	CA	GLY	687	50.051	2.603	24.286	1.00 30.57
MOTA	3721	C	GLY		48.758	1.939	24.273	1.00 31.78
ATOM	3722	0	GLY	687	48.202	1.923	22.862	1.00 32.51
ATOM	3723	N	VAL	687	47.687	0.908	22.373	1.00 31.25
ATOM	3724	CA	VAL	688	48.292	3.073	22.204	1.00 32.58
ATOM	3725	СВ	VAL	688	47.825	3.202	20.827	1.00 30.66
ATOM	3726	CG1		688	47.804	4.684	20.362	1.00 28.55
ATOM	3727	CG2		688	47.231	4.795	18.950	1.00 27.25
ATOM	3728		VAL	688	46.944	5.522	21.320	1.00 27.12
ATOM	3729			688	48.684	2.326	19.910	1.00 29.96
ATOM	3730		VAL	688	48.160	1.731	18.974	1.00 30.83
ATOM	3731		LEU	689	49.973	2.202		1.00 30.02
ATOM	3732		LEU	689	50.893	1.371		1.00 30.48
ATOM			LEU	689	52.359	1.571		1.00 28.13
MOTA	3733 3734		LEU	689	53.466	0.966		1.00 26.34
ATOM		CD1		689	54.790	1.697		1.00 25.54
		CD2		689	53.628	-0.505		1.00 24.99
			LEU	689	50.479	-0.096		1.00 30.54
			LEU	689	50.540	-0.849		1.00 27.86
	3738	N I	LEU	690	50.013			1.00 33.73

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ATOM 3739 CA LEU 690 49.553 -1.830 21.029 1.00 32.47 MOTA 3740 CB 690 LEU 49.141 -1.982 22.496 1.00 31.82 ATOM 3741 CG LEU 690 50.135 -2.220 23.634 1.00 29.71 **ATOM** 3742 CD1 LEU 690 49.396 -2.129 24.956 1.00 31.53 3743 MOTA CD2 LEU 690 50.771 -3.605 23.483 1.00 31.69 ATOM 3744 C LEU 690 48.335 -2.101 20.136 1.00 33.01 MOTA 3745 0 LEU 690 48.223 -3.168 19.521 1.00 32.68 ATOM 3746 N. TRP 691 47.423 -1.131 20.089 1.00 32.37 **ATOM** 3747 CA TRP 691 -1.215 46.230 19.256 1.00 32.11 **ATOM** 3748 CB TRP 691 45.424 0.083 19.373 1.00 33.19 **ATOM** 3749 CG TRP 691. 44.086 0.055 18.678 1.00 33.95 MOTA 3750 CD2 TRP 691 43.812 0.469 17.337 1.00 30.48 MOTA 3751 CE2 TRP 691 42.434 0.294 17.118 1.00 32.75 MOTA 3752 CE3 TRP 691 44.599 0.989 16.301 1.00 29.47 MOTA 3753 CD1 TRP 691 42.889 -0.352 19.199 1.00 34.34 NE1 TRP **ATOM** 3754 691 41.894 -0.211 18.272 1.00 36.53 0.601 **ATOM** 3755 CZ2 TRP 691 41.831 15.900 1.00 30.85 **ATOM** 3756 CZ3 TRP 691 44.003 1.289 15.100 1.00 30.51 MOTA 3757 CH2 TRP 691 42.630 1.104 1.4.907 1.00 30.29 MOTA 3758 C TRP 691 46.661 -1.421 17.805 1.00 31.49 ATOM 3759 0 TRP 691 46.062 -2.221 17.092 1.00 31.20 ATOM 3760 N GLU 692 47.669 -0.656 17.374 1.00 32.90 ATOM 3761 CA GLU 692 48.207 -0.734 16.019 1.00 29.78 **ATOM** 3762 CB GLU 692 49.383 0.233 15.809 1.00 25.56 ATOM 3763 CG GLU 692 49.009 1.696 15.713 1.00 25.85 MOTA 3764 CD GLU 692 50.195 2.570 15.363 1.00 27.76 **ATOM** 3765 OE1 GLU 692 51.001 2.850 16.265 1.00 29.52 **ATOM** 3766 OE2 GLU 692 50.333 2.981 14.191 1.00 26.84 MOTA 3767 C GLU 692 48.682 -2.136 15.696 1.00 31.08 **ATOM** 3768 0 GLU 692 48.545 -2.593 1.00 32.57 14.553 MOTA 3769 ILE -2.804 N 693 49.262 16.689 1.00 31.81 MOTA 3770 CA ILE 693 49.774 -4.163 16.506 1.00 31.87 ATOM 3771 CB ILE 693 -4.614 50.666 17.699 1.00 33.50 MOTA 3772 CG2 ILE 693 51.140 -6.075 17.513 1.00 33.06 **ATOM** 3773 CG1 ILE 693 51.879 -3.703 17.827 1.00 34.04 **ATOM** 3774 CD1 ILE 693 52.744 -4.008 19.025 1.00 31.52 ATOM 3775 C ILE 693 48.643 -5.177 16.335 1.00 31.43 **ATOM** 3776 0 ILE 693 48.633 -5.982 15.403 1.00 29.55 **ATOM** 3777 N PHE 694 47.654 -5.087 17.207 1.00 33.58 ATOM 3778 CA PHE 694 46.550 -6.027 17.178 1.00 36.72 **ATOM** 3779 CB PHE 694 45.980 -6.179 18.589 1.00 36.27 **ATOM** 3780 CG PHE 694 46.988 -6.724 19.547 1.00 34.29 **ATOM** 3781 CD1 PHE 694 47.500 -5.949 20.581 1.00 34.95 MOTA 3782 CD2 PHE -7.972 694 47.560 19.297 1.00 31.60 ATOM 3783 CE1 PHE 694 -6.413 48.576 21.344 1.00 35.73 ATOM 3784 CE2 PHE 694 48.633 -8.443 20.049 1.00 31.12 MOTA 3785 CZPHE 694 49.149 -7.661 21.066 1.00 33.97 MOTA 3786 С PHE 694 45.516 -5.870 16.065 1.00 37.70 MOTA 3787 0 PHE 694 44.684 -6.756 15.839 1.00 37.99 MOTA 3788 N THR 695 45.604 -4.745 15.355 1.00 36.11 MOTA 3789 CA THR 695 44.747 -4.485 14.205 1.00 31.23 ATOM 3790 CB THR 695 44.107 -3.081 14.236 1.00 30.49

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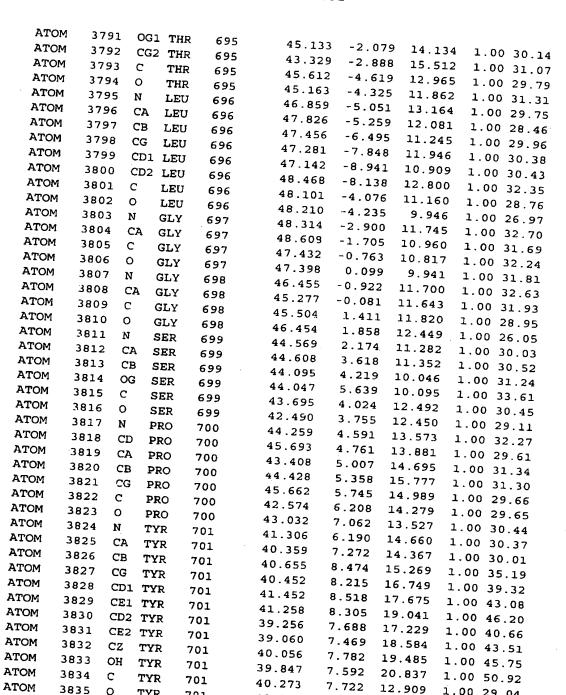
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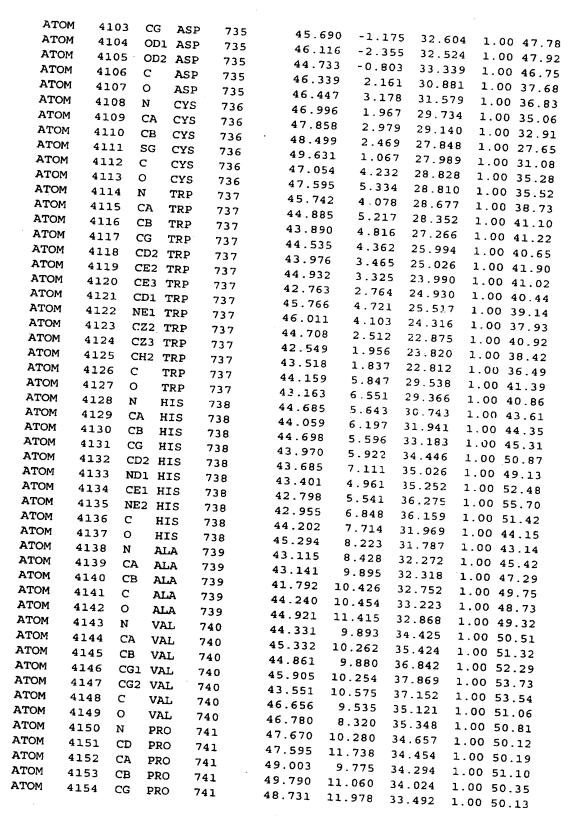
ATOM 3843 GLY N 703 39.148 9.213 9.591 1.00 28.34 **ATOM** 3844 CA GLY 703 38.191 10.236 9.226 1.00 25.97 ATOM 3845 C GLY 703 37.960 11.289 10.297 1.00 28.00 **ATOM** 3846 GLY 0 703 37.175 12.213 10.079 1.00 26.40 ATOM 3847 VAL N 704 38.621 11.139 11.448 1.00 29.54 **ATOM** 3848 CA VAL 704 38.480 12.061 12.576 1.00 30.61 ATOM 3849 CB VAL 704 38.606 11.324 13.944 1.00 32.54 ATOM 3850 CG1 VAL 704 38.577 12.324 15.111 1.00 31.95 **ATOM** 3851 CG2 VAL 704 37.482 10.311 14.103 1.00 34.62 MOTA 3852 С VAL 704 39.490 13.210 12.557 1.00 31.37 MOTA 3853 0 VAL 704 40.683 13.001 12.757 1.00 31.73 MOTA 3854 N PRO 705 39.030 14.430 12.281 1.00 32.70 **ATOM** 3855 PRO CD 705 37.669 14.770 11.819 1.00 33.75 **ATOM** 3856 CA PRO 705 39.910 15.599 12.243 1.00 31.90 **ATOM** 3857 CB PRO 705 39.065 16.641 11.518 1.00 32.66 **ATOM** 3858 CG PRO 705 37.674 16.273 11.906 1.00 35.32 **ATOM** 3859 С PRO 705 40.331 16.053 13.635 1.00 31.85 **ATOM** 3860 О PRO 705 39.709 15.686 14.634 1.00 31.50 ATOM 3861 N VAL 706 41.372 16.879 13.676 1.00 32.32 **ATOM** 3862 CA VAL 706 41.945 17.389 14.925 1.00 36.88 **ATOM** 3863 CB VAL 706 42.991 18.505 14.664 1.00 39.77 MOTA 3864 CG1 VAL 706 43.657 18.907 15.974 1.00 39.17 MOTA 3865 CG2 VAL 706 44.035 18.057 13.618 1.00 38.70 MOTA 3866 C VAL 706 40.938 17.923 15.953 1.00 37.80 MOTA 3867 0 VAL 706 40.994 17.581 17.140 1.00 37.45 MOTA 3868 N GLU 707 39.991 18.724 15.483 1.00 38.19 MOTA 3869 CA GLU 707 39.009 19.308 16.370 1.00 37.31 **ATOM** 3870 CB GLU 707 38.208 20.361 15.619 1.00 37.46 ATOM 3871 C GLU 707 38.084 18.264 16.994 1.00 39.56 MOTA 3872 0 GLU 707 37.739 18.344 18.177 1.00 41.39 ATOM 3873 N GLU 708 37.724 17.260 16.206 1.00 39.99 **ATOM** 3874 CA GLU 708 36.840 16.212 16.684 1.00 40.08 **ATOM** 3875 СB GLU 708 36.334 15.377 15.515 1.00 43.96 MOTA 3876 CG GLU 708 35.505 16.163 14.496 1.00 46.61 **ATOM** 3877 CD GLU 708 34.288 16.851 15.099 1.00 52.77 **ATOM** 3878 OE1 GLU 708 33.659 16.305 16.040 1.00 52.52 ATOM 3879 OE2 GLU 708 33.954 17.955 14.604 1.00 57.04 **ATOM** 3880 С GLU 708 37.551 15.337 17.704 1.00 39.89 ATOM 3881 0 GLU 708 36.944 14.900 18.684 1.00 39.47 ATOM 3882 N LEU 709 38.838 15.086 17.471 1.00 38.99 ATOM 3883 CA LEU 709 39.638 14.277 18.393 1.00 37.51 **ATOM** 3884 CB LEU 709 41.079 14.120 17.892 1.00 34.15 **ATOM** 3885 LEU CG 709 42.061 13.338 18.787 1.00 30.94 MOTA 3886 CD1 LEU 709 41.861 11.834 18.689 1.00 28.48 MOTA 3887 CD2 LEU 709 43.459 13.712 18.395 1.00 29.02 **ATOM** 3888 C LEU 709 39.644 14.961 19.751 1.00 38.18 **ATOM** 3889 0 LEU 709 39.460 14.313 20.787 1.00 38.08 **ATOM** 3890 N PHE 710 39.833 16.276 1.00 39.68 19.749 MOTA 3891 CA PHE 710 39.845 17.021 21.001 1.00 43.27 **ATOM** 3892 CB PHE 710 40.024 18.524 20.747 1.00 43.66 MOTA 3893 CG PHE 710 41.376 18.888 20.225 1.00 46.36 ATOM 3894 CD1 PHE 710 42.459 18.024 20.403 1.00 48.33

ATOM		95 (	CD2 PH	E 710	41.5	70 20 0		
ATON	1 389		CE1 PH		43.7	_		
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ATOM	390	0 0			38.55			
ATOM	390	1 N			38.58		_	
ATOM	390	2 C	A LY		37.44			1.00 45.27
MOTA	390	3 C			36.14		- <del>-</del> ·	
ATOM	390	4 C			35.03			1.00 46.68
ATOM	390	5 C			33.64			1.00 52.36
ATOM	390	6 CI			32.55			1.00 54.43
ATOM	390	7 N			31.19			1.00 55.93
MOTA	390	в с	LYS	·	30.10			1.00 63.51
MOTA	3909	9 0	LYS		36.05			1.00 42.15
ATOM	3910		LEU		35.63			1.00 40.85
ATOM	3911				36.46			1.00 40.98
ATOM	3912				36.43			1.00 42.26
ATOM	3913				37.012			1.00 39.67
MOTA	3914	CD	1 LEU		36.159			1.00 39.06
ATOM	3915			712	36.899	_		1.00 36.97
ATOM	3916		LEU	712	34.842			1.00 36.48
MOTA	3917	0	LEU	712	37.232			1.00 43.61
ATOM	3918	N	LEU	713	36.796	_		1.00 44.10
ATOM	3919		LEU	713	38.407	_	23.038	1.00 43.57
MOTA	3920	СВ	LEU	713	39.271		24.207	1.00 43.67
ATOM	3921	CG	LEU	713	40.619		23.958	1.00 42.24
ATOM	3922		LEU	713	41.569		22.989	1.00 38.81
ATOM	3923		LEU	713	42.856		22.817	1.00 30.86
ATOM	3924	С	LEU	713	41.873		23.519	1.00 34.27
ATOM	3925	0	LEU	713	38.589	13.594	25.450	1.00 44.78
ATOM	3926	N	LYS	714	38.548	12.919	26.472	1.00 46.04
ATOM	3927	CA	LYS	714	38.002	14.785	25.344	1.00 44.72
ATOM	3928	CB	LYS	714	37.304	15.394	26.471	1.00 44.34
ATOM	3929	CG	LYS	714	36.818	16.799	26.114	1.00 43.76
ATOM	3930	CD	LYS	714	37.955	17.761	25.926	1.00 46.37
MOTA	3931	CE	LYS	714	37.497	19.174	25.628	1.00 52.22
ATOM	3932	NZ	LYS	714	38.701	20.044	25.235	1.00 57.37
MOTA	3933	С	LYS	714	39.792	20.059	26.279	1.00 58.02
ATOM	3934	0	LYS	714	36.142	14.534	26.972	1.00 44.17
ATOM	3935	N	GLU	715	35.861	14.499	28.167	1.00 45.14
ATOM	3936	CA	GLU	715	35.498	13.809	26.068	1.00 43.86
ATOM	3937	CB	GLU		34.392	12.935	26.430	1.00 42.94
ATOM	3938	CG	GLU	715	33.518	12.652	25.195	1.00 46.57
ATOM	3939	CD	GLU	715	32.930	13.897	24.532	1.00 51.37
ATOM	3940	OE1		715	32.032	13.571	23.338	1.00 54.24
ATOM	3941	OE2		715	32.215	12.503	22.704	1.00 54.19
ATOM	3942	C		715	31.139	14.392	23.033	1.00 55.01
ATOM	3943		GLU	715	34.878	11.607		1.00 41.36
	3944		GLU	715	34.076	10.730		.00 38.24
	3945		GLY	716	36.184	11.452		.00 41.41
	3946		GLY	716	36.727			.00 41.78
<b>-</b>	-240	C	GLY	716	36.602			.00 42.65
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MOTA	3947	0	GLY	716	36.661	7.874	27.225	1.00 41.41
ATOM	3948	N	HIS	717	36.439	9.321	25.513	1.00 44.56
ATOM	3949	CA	HIS	717	36.286	8.291	24.502	1.00 45.91
ATOM	3950	CB	HIS	717	35.935	8.926	23.153	1.00 46.65
ATOM	3951	CG	HIS	717	35.860	7.946	22.024	1.00 50.03
ATOM	3952	CD2	HIS	717	34.842	7.171	21.581	1.00 49.92
MOTA	3953		HIS	717	36.946	7.634	21.235	1.00 51.38
MOTA	3954		HIS	717	36.604	6.708	20.360	1.00 50.10
MOTA	3955	NE2	HIS	717	35.335	6.408	20.550	1.00 49.34
MOTA	3956	С	HIS	717	37. <b>5</b> 35	7.434	24.354	1.00 47.68
ATOM	3957	0	HIS	717	38.649	7.949	24.287	1.00 49.77
MOTA	3958	N	ARG	718	37.328	6.118	24.283	1.00 48.18
MOTA	3959	CA	ARG	718	38.403	5.148	24.116	1.00 46.95
ATOM	3960	CB	ARG	718	38.571	4.307	25.385	1.00 45.75
ATOM	3961	CG	ARG	718	38.945	5.125	26.618	1.00 47.15
ATOM	3962	CD	ARG	718	40.273	5.852	26.420	1.00 46.61
ATOM	3963	NE	ARG	718	40.722	6.579	27.608	1.00 45.57
ATOM	3964	CZ	ARG	718	40.601	7.896	27.779	1.00 45.48
MOTA	3965		ARG	718	40.033	8.644	26.845	1.00 44.14
ATOM	3966		ARG	718	41.122	8.480	28.854	1.00 43.32
ATOM	3967	C	ARG	718	38.109	4.250	22.912	1.00 47.56
ATOM	3968	Ò	ARG	718	36.946	3.991	22.589	1.00 48.37
ATOM	3969	N	MET	719	39.149	3.873	22.181	1.00 47.33
ATOM	3970	CA	MET	719	38.984	3.021	21.013	1.00 47.90
ATOM	3971	CB	MET	719	40.282	2.939	20.198	1.00 47.21
ATOM	3972	CG	MET	719	40.652	4.245	19.509	1.00 45.79
ATOM	3973	SD	MET	719	42.095	4.104	18.440	1.00 42.81
ATOM	3974	CE	MET	719	43.377	3.970	19.604	1.00 43.02
ATOM	3975	C	MET	719	38.519	1.629	21.392	1.00 49.99
ATOM	3976	0	MET	719	38.889	1.102	22.450	1.00 47.98
ATOM	3977	N	ASP	720	37.690	1.050	20.523	1.00 53.40
ATOM ATOM	3978	CA	ASP	720	37.135	-0.288	20.722	1.00 53.19
ATOM	3979 3980	CB CG	ASP	720	36.089	-0.638	19.647	1.00 56.95
MOTA	3981	OD1	ASP	720 · 720	34.916	0.333	19.605	1.00 61.65
ATOM	3982	OD2		720	34.908	1.331	20.356	1.00 68.60
ATOM	3983	C	ASP	720	33.996	0.095	18.792	1.00 61.19
ATOM	3984	0	ASP	720	38.208	-1.372	20.713	1.00 51.12
MOTA	3985	N	LYS	720	39.263	-1.229	20.081	1.00 50.71
ATOM	3986	CA	LYS	721	37.926 38.833	-2.453	21.432	1.00 48.85
ATOM	3987	CB	LYS	721	38.335	-3.576 -4.560	21.509	1.00 47.92
ATOM	3988	CG	LYS	721	39.024	-5.901	22.562 22.521	1.00 47.79 1.00 51.08
ATOM	3989	CD	LYS	721	38.493	-6.810	23.597	1.00 51.08
ATOM	3990	CE	LYS	721	38.484	-8.255	23.141	1.00 54.60
MOTA	3991	NZ	LYS	721	38.158	-9.176	24.268	1.00 54.60
ATOM	3992	C	LYS	721	38.861	-4.261		
ATOM	3993	0	LYS	721	37.822	-4.688	20.155	1.00 49.01
ATOM	3994	N	PRO	722	40.053	-4.366	19.653 19.541	1.00 52.79
ATOM	3995	CD	PRO	722	41.356	-3.839	19.541	1.00 48.92 1.00 51.11
ATOM	3996	CA	PRO	722	40.167	-5.011	18.233	1.00 46.01
ATOM	3997	CB	PRO	722	41.663	-4.904	17.918	1.00 45.61
ATOM	3998	CG	PRO	722	42.090	-3.690	18.646	1.00 45.84
					12.000	3.000	10.040	1.00 1/.00

ATC			C PR	20 722	39.745 -6.466 18.303 1 00 43 57
ATO			O PR	0 722	39 710 10.303 1.00 43.57
ATO			n se	R 723	20 260 - 1.00 41.72
ATO	<del>-</del>		CA SE	R 723	38 991 0 300 1.00 43.14
ATO:	- •		CB SE		38 360 0 555
ATO	. •	04 (	OG SE		39 112 0 404
ATO	M 400	05 (	SE		40 330
ATO	M 400	06 (	SE		1.00 41.68
ATO	M 400	7 1	I ASI		41.299 -8.605 16.493 1.00 40.84
ATON	400	)8 C	A ASI		40.405 -10.275 17.683 1.00 45.99
ATOM	400	9 0	B ASN		12.031 -11.034 17.800 1.00 49.22
ATOM	1 401	.o c	G ASN		42.342 -11.215 16.453 1.00 52.35
ATOM			D1 ASN		41.768 -12.357 15.668 1.00 58.07
ATOM			D2 ASN		41.021 -13.506 16.103 1.00 62 42
ATOM	401				41.186 ~12.054 14.513 1 00 62 13
ATOM				- <del>-</del>	42.558 -10.323 18.787 1.00 49.77
ATOM		_			43.698 -9.982 18.494 1 00 51 40
ATOM					41.995 -10.054 19.954 1 00 50 34
ATOM					42.698 -9.398 21.028 1 60 49 83
MOTA	4018				42.623 -7.878 20.868 1.00 47 11
ATOM	4019				43.485 -6.992 22.169 1 00 30 55
ATOM	4020		CYS	725	42.001 -9.861 22.299 1.00 50 11
ATOM	4021	_	CYS	725	40.772 -9.852 22.383 1.00 50 63
ATOM	4022		THR	726	42.788 -10.350 23.244 1.00 50.37
ATOM	4023			726	42.261 -10.843 24.497 1.00 51.05
ATOM	4023			726	43 341 71 663
ATOM	4025		1 THR	726	44 292 -10 700 05
ATOM	4025			726	44.074 -12.554 24.241 1.00 52.55
ATOM	4025		THR	726	41.843 -9.665 25.354 1.00 52.18
ATOM	4027		THR	726	42.403 -8.574 25.219 1.00 55.14
ATOM			ASN	727	40.868 -9.860 26.237 1.00 52.55
ATOM	4029 4030		ASN	727	40.401 -8.781 27.114 1.00 53.17
ATOM		CB	ASN	727	39.246 -9.265 27.992 1.00 60.65
ATOM	4031	CG	ASN	727	39.584 -10.545 28.751 1.00 68.99
ATOM	4032		L ASN	727	40 704 10 77
MOTA	4033		2 ASN	727	39 630 77
ATOM	4034	C	ASN	727	41 527 6 55
ATOM	4035	0	ASN	727	41 512 5 50.79
ATOM	4036	N	GLU	728	42 522 0 000
	4037	CA	GLU	728	43 603
ATOM ATOM	4038	CB	GLU	728	44 544 10 000
	4039	CG	GLU	728	45 003
ATOM	4040	CD	GLU	728	45 500 35 35 35 35 35 35 35 35 35 35 35 35 35
ATOM	4041		GLU	728	46 777 10 50.45
ATOM	4042	OE2	GLU	728	46 005 33.73
MOTA	4043	C	GLU	728	44 500 57.38
ATOM	4044	0	GLU	728	44 760 6 6 6 6 92
ATOM	4045	N	LEU	729	44 860
ATOM	4046	CA	LEU	729	45 643 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7
ATOM	4047	CB	LEU	729	45 050 7 7 7 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
ATOM	4048	CG	LEU	729	47 004
ATOM	4049		LEU	729	15 000 34.35
ATOM	4050	CD2		729	10 101
			-		48.404 -8.320 25.139 1.00 33.63

MOTA	4051	С	LEU	729	44.909	-5.817	25.985	1.00	40.58
ATOM	4052	0	LEU	729	45.524	-4.760	25.929	1.00	40.10
MOTA	4053	N	TYR	730	43.591	-5.886	25.917	1.00	39.32
ATOM	4054	CA	TYR	730	42.807	-4.694	25.720	1.00	41.49
MOTA	4055	CB	TYR	730	41.384	-5.052	25.302	1.00	39.70
ATOM	4056	CG	TYR	730	40.507	-3.846	25.099	1.00	39.53
ATOM	4057	CD1	TYR	730	40.828	-2.879	24.142	1.00	35.10
MOTA	4058	CE1	TYR	730	40.019	-1.758	23.958	1.00	36.33
ATOM	4059	CD2	TYR	730	39.352	-3.661	25.874	1.00	38.44
ATOM	4060	CE2	TYR	730	38.537	-2.541	25.696	1.00	37.68
ATOM	4061	CZ	TYR	730	38.876	-1.601	24.730	1.00	36.85
MOTA	4062	OH	TYR	730	38.041	-0.541	24.489	1.00	40.58
ATOM	4063	C	TYR	730	42.814	-3.849	26.993	1.00	43.50
ATOM	4064	0	TYR	730	42.880	-2.621	26.931	1.00	44.45
ATOM	4065	N	MET	731	42.753	-4.492	28.151	1.00	46.53
MOTA	4066	CA	MET	731	42.782	-3.744	29.406	1.00	48.67
MOTA	4067	СВ	MET	731	42.488	-4.668	30.590	1.00	54.90
MOTA	4068	CG	MET	731	41.072	-5.229	30.577	1.00	63.75
MOTA	4069	SD	MET	731	39.766	-3.998	30.763	1.00	69.82
MOTA	4070	CE	MET	731	39.849	-3.788	32.581	1.00	68.20
ATOM	4071	С	MET	731	44.148	-3.087	29.551	1.00	45.73
ATOM	4072	0	MET	731	44.273	-2.024	30.160	1.00	42.09
MOTA	4073	И	MET	732	45.168	-3.728	28.986	1.00	43.47
ATOM	4074	CA	MET	732	46.519	-3.189	29.024		43.85
ATOM	4075	CB	MET	732	47.515	-4.154	28.365	1.00	40.67
ATOM	4076	CG	MET	732	48.966	-3.646	28.369	1.00	39.96
ATOM	4077	SD	MET	732	50.252	-4.870	27.887	1.00	35.34
ATOM	4078	CE	MET	732	50.523	-5.667	29.390		35.15
ATOM	4079	C	MET	732	46.460	-1.860	28.275		43.91
ATOM	4080	0	MET	732	46.924	-0.835	28.782		47.29
ATOM	4081	N	MET	733	45.798	-1.860	27.120		42.51
ATOM	4082	CA	MET	733	45.639	-0.652	26.319		39.85
ATOM	4083	CB	MET	733	44.888	-0.932	25.013		38.08
ATOM ATOM	4084	CG	MET	733	45.614	-1.805	23.991		37.14
MOTA	4085	SD	MET	733	44.509	-2.170	22.578		37.32
ATOM	4086	CE	MET	733	45.198	-3.684	21.929		28.98
ATOM	4087 4088	0	MET MET	733 733	44.838	0.363	27.123		41.12
ATOM	4089	N	ARG	734	45.228	1.532	27.213		44.38
ATOM	4090	CA	ARG	734	43.737		27.731	1.00	
ATOM	4091	CB	ARG	734	42.893 41.632	0.813 0.095	28.516 29.007	1.00	
ATOM	4092	CG	ARG	734	40.723	-0.384		1.00	
ATOM	4093	CD	ARG	734	40.723	0.741	27.894 26.995	1.00	
ATOM	4094	NE	ARG	734	39.510	1.733	27.682	1.00	
ATOM	4095	cz	ARG	734	38.182	1.681	27.774	1.00	
ATOM	4096		ARG	734	37.503	0.681	27.774	1.00	
ATOM	4097	NH2	ARG	734	37.526	2.633	28.416		
ATOM	4098	C	ARG	734	43.694	1.387	29.675	1.00	
ATOM	4099	0	ARG	734	43.538	2.564	30.010	1.00	
ATOM	4100	N	ASP	735	44.583	0.572	30.010	1.00	
ATOM	4101	CA	ASP	735	45.465	1.000	31.339	1.00	
ATOM	4102	CB	ASP	735	46.392	-0.137	31.773	1.00	
		. –		- <del>-</del>			J = . , . J		-2.50



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MOTA 4155 C PRO 741 49.687 8.902 35.340 1.00 52.02 ATOM 4156 PRO 741 0 50.374 7.941 34.998 1.00 50.79 **ATOM** 4157 N SER 742 49.482 9.228 36.613 1.00 53.75 **ATOM** 4158 CA SER 742 50.079 8.474 37.708 1.00 54.58 **ATOM** 4159 CB SER 742 49.921 9.245 39.020 1.00 57.25 ATOM 4160 OG SER 742 48.572 1.00 61.69 9.629 39.237 ATOM 4161 С SER 742 49.479 7.077 37.851 1.00 53.33 MOTA 4162 0 SER 742 50.074 6.189 38.464 1.00 52.98 ATOM 4163 N GLN 743 48.286 6.897 37.305 1.00 52.97 MOTA 4164 CA GLN 743 47.616 5.613 37.390 1.00 52.15 MOTA 4165 CB GLN 743 46.108 5.827 37.505 1.00 56.12 ATOM 4166 CG GLN 743 45.506 5.374 38.838 1.00 60.50 ATOM 4167 CD GLN 743 46.269 5.887 40.046 1.00 64.45 MOTA 4168 OE1 GLN 743 46.910 5.114 40.752 1.00 65.64 ATOM 4169 NE2 GLN 743 46.199 7.194 40.290 1.00 67.99 **ATOM** 4170 C GLN 743 47.963 4.690 36.229 1.00 49.54 MOTA 4171 0 GLN 743 47.629 3.499 36.246 1.00 50.07 **ATOM** 4172 N ARG 744 48.605 5.241 35.202 1.00 46.93 **ATOM** 4173 ARG CA 744 49.010 4.437 34.044 1.00 44.51 ATOM 4174 CBARG 744 49.478 5.330 32.894 1.00 39.30 ATOM 4175 CG ARG 744 48.433 6.300 32.360 1.00 32.53 **ATOM** 4176 CD ARG 744 48.991 7.178 31.254 1.00 25.50 ATOM 4177 NE ARG 744 48.034 8.218 30.932 1.00 32.16 **ATOM** 4178 CZARG 744 48.352 9.454 30.542 1.00 34.35 MOTA 4179 NH1 ARG 744 49.622 9.814 30.400 1.00 30.49 MOTA 4180 NH2 ARG 744 47.382 10.349 30.350 1.00 32.23 MOTA 4181 С ARG 744 50.153 3.498 34.472 1.00 44.61 ATOM 4182 0 ARG 744 50.833 3.741 35.474 1.00 47.68 **ATOM** 4183 N PRO 745 50.319 2.365 33.765 1.00 43.21 ATOM 4184 CD PRO 745 49.444 1.737 32.763 1.00 42.00 **ATOM** 4185 CA PRO 745 51.414 1.470 34.157 1.00 40.11 **ATOM** 4186 CB PRO 745 51.004 0.132 33.532 1.00 37.54 MOTA 4187 CG PRO 745 50.251 0.515 32.335 1.00 36.49 **ATOM** 4188 C PRO 745 52.744 1.956 33.612 1.00 39.15 **ATOM** 4189 0 PRO 745 52.807 2.654 32.602 1.00 40.56 MOTA 4190 THR N 746 53.812 1.626 34.316 1.00 37.77 MOTA 4191 CA THR 746 55.135 2.020 33.886 1.00 37.61 ATOM 4192 CB THR 746 56.113 2.132 35.091 1.00 39.14 ATOM 4193 OG1 THR 746 56.439 0.824 1.00 35.16 35.600 MOTA 4194 CG2 THR 746 55.489 2.990 36.195 1.00 36.82 ATOM 4195 C THR 746 55.687 1.036 32.852 1.00 36.75 4196 MOTA 0 THR 746 1.00 32.89 55.228 -0.103 32.772 ATOM 4197 N PHE 747 56.649 1.482 32.043 1.00 36.56 **ATOM** 4198 CA PHE 747 57.267 0.599 31.055 1.00 33.79 ATOM 4199 CB PHE 747 58.305 1.350 30.226 1.00 28.85 **ATOM** 4200 CG PHE 747 57.702 2.123 29.103 1.00 30.71 **ATOM** 4201 CD1 PHE 747 57.060 1.455 28.059 1.00 26.42 MOTA 4202 CD2 PHE 747 57.749 3.510 29.080 1.00 28.73 ATOM 4203 CE1 PHE 747 56.469 2.154 27.025 1.00 26.56 MOTA 4204 CE2 PHE 747 57.150 4.216 28.047 1.00 28.97 **ATOM** 4205 CZPHE 747 56.518 3.535 27.018 1.00 28 95 **ATOM** 4206 С PHE 747 57.901 -0.593 31.732 1.00 34.64

ATO:	M 42	07	O PI	ID 2.5				
ATO					58.00		7 31.156	1.00 31.47
ATO					58.328		32.972	1.00 38.86
ATO			CA LY		58.92(			
ATO			CB LY		59.529	-0.952		
ATON			CG LY		60.200	-2.047		
			CD LY		60.917			
ATON			CE LY	S 748	61.353			1.00 51.33
ATOM			NZ LY	S 748	62.135			1.00 51.17
ATOM			C LY	S 748	57.813			1.00 56.55
ATOM			LY:	S 748	58.025			1.00 41.14
ATOM		L7 1	V GL		56.622		=	1.00 38.24
ATOM		18 (	A GL		55.454		34.383	1.00 41.20
ATOM		.9 0	B GLM		54.254	-2.856	34.669	1.00 40.49
ATOM		0 C	G GLN			-2.015	35.134	1.00 45.70
ATOM	422	1 0	D GLN		54.378	-1.368	36.500	1.00 50.61
ATOM	422		E1 GLN		53.203	-0.441	36.797	1.00 55.26
ATOM	422		E2 GLN		53.392	0.727	37.123	1.00 58.00
MOTA	422			_	51.988	-0.951	36.665	1.00 59.25
ATOM	422	_			55.049	-3.588	33.397	1.00 37.42
ATOM	422	-			54.964	-4.810	33.369	1.00 36.00
ATOM	422			•	54.810	-2.817	32.340	1.00 36.76
ATOM	422				54.409	-3.355	31.033	1.00 35.39
MOTA	422				54.358	-2.241	29.984	1.00 30.97
ATOM	423				53.369	-1.091	30.177	1.00 27.36
ATOM			ol LEU	750	53.745	0.037	29.217	
ATOM	4233			750	51.941	-1.578	29.934	1.00 29.15 1.00 29.22
ATOM	4232	_	LEU	750	55.369	-4.437	30.557	1.00 29.22
ATOM	4233	_	LEU	750	54.934	-5.449	30.014	
ATOM	4234		VAL	751	56.673	-4.212		1.00 34.45
	4235			751	57.656	-5.217		1.00 38.76
ATOM	4236			751	59.129	-4.724		1.00 38.69
ATOM	4237		1 VAL	751	60.092	-5.836		1.00 33.81
ATOM	4238	CG	2 VAL	751	59.415		_	1.00 32.04
MOTA	4239	C	VAL	751	57.428			1.00 30.67
ATOM	4240	0	VAL	751	57.492		31.131	1.00 41.68
ATOM	4241	N	GLU	752	57.109			1.00 39.92
ATOM	4242	CA	GLU	752	56.854			1.00 44.22
ATOM	4243	CB	GLU	752				1.00 47.43
ATOM	4244	CG	GLU	752				L.00 49.29
ATOM	4245	CD	GLU	752			35.212 1	1.00 53.53
MOTA	4246	OE:	LGLU	752			36.707 1	.00 53.05
ATOM	4247		GLU	752			37.136 1	00 53.63
ATOM	4248	C	GLU	752 752			37.452 1	00 56.18
ATOM	4249	0	GLU			-8.256	32.809 1	.00 46.90
ATOM	4250	N	ASP	752 753		-9.464 3	32.551 1	.00 43.85
ATOM	4251	CA		753		-7.529 3	32.640 1	.00 48.05
ATOM	4252		ASP	753	53.232			.00 48.46
ATOM	4253	CB	ASP	753	52.119 -			.00 51.25
ATOM		CG	ASP	753	51.579 -			.00 54.20
ATOM	4254		ASP	753				.00 57.31
	4255		ASP	753				00 57.31
ATOM	4256	С	ASP	753				.00 55.58
MOTA	4257	0	ASP	753				.00 48.59
MOTA	4258	N	LEU	754				.00 49.69
							9.889 1.	.00 47.21

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MOTA	4259	CA	LEU	754	54.102	-8.489	28.523	1.00	46.37
MOTA	4260	CB	LEU	754	54.664	-7.385	27.625	1.00	44.16
ATOM	4261	CG	LEU	754	53.621	-6.366	27.152	1.00	46.35
ATOM	4262		LEU		54.296	-5.272	26.343	1.00	45.11
MOTA	4263		LEU	754	52.514	-7.070	26.349	1.00	42.89
ATOM	4264	С	LEU	754	55.004	-9.703	28.481	1.00	47.08
MOTA	4265	0	LEU	754	54.818	-10.590	27.659	1.00	45.02
ATOM	4266	N	ASP	755	55.969	-9.755	29.385	1.00	49.68
ATOM	4267	CA	ASP	755	56.890	-10.876	29.487	1.00	51.62
ATOM	4268	CB	ASP	755	57.883	-10.586	30.615	1.00	54.90
MOTA	4269	CG	ASP	755	59.009	-11.589	30.702	1.00	59.00
ATOM	4270		ASP	755	59.694	-11.608	31.746	1.00	63.70
MOTA	4271		ASP	755	59.223	-12.346	29.728	1.00	60.31
ATOM	4272	С	ASP	755	56.059	-12.117	29.817	1.00	51.50
ATOM	4273	0	ASP	755	56.119	-13.150	29.138	1.00	47.11
ATOM	4274	N	ARG	756	55.237	-11.958	30.844	1.00	51.81
ATOM	4275	CA	ARG	756	54.362	-13.009	31.328	1.00	51.44
ATOM	4276	CB	ARG	756		-12.519	32.582	1.00	54.52
ATOM	4277	CG	ARG	756		-13.358	33.027	1.00	55.00
ATOM	4278	CD	ARG	756	_	-12.727	34.255	1.00	59.54
ATOM	4279	NE	ARG	756		-11.335	34.026		64.01
ATOM	4280	CZ	ARG	756		-10.960	33.301	1.00	
ATOM	4281		ARG	756	49.598	-11.866	32.721	1.00	63.56
ATOM	4282		ARG	756	50.061	-9.676	33.183	1.00	66.59
ATOM	4283	C	ARG	756		-13.440	30.260	1.00	50.03
ATOM ATOM	4284	0	ARG	756 757		-14.622	29.960		49.98
ATOM	4285 4286	N CA	ILE	757 757		-12.483	29.673		46.87
ATOM	4287	CB	ILE	757 757		-12.789	28.644		44.28
ATOM	4288	CG2		757 757		-11.532	28.125		40.46
ATOM	4289	CG1		757		-11.923	27.062	1.00	
ATOM	4290		ILE	757	49.481	-10.830 -9.551	29.277	1.00	39.74
ATOM	4291	C	ILE	757	52.251	-13.528	28.920 27.454		40.68
ATOM	4292	ō	ILE	757		-14.469	26.959		40.28
ATOM	4293	N	VAL	758		-13.111	27.014		47.56
ATOM	4294	CA	VAL	758		-13.745	25.874		48.90
ATOM	4295	CB	VAL	758		-13.177	25.609		47.01
ATOM	4296		VAL	758		-13.920	24.456		44.38
ATOM	4297	CG2	VAL	758		-11.714	25.262		47.85
ATOM	4298	C	VAL	758		-15.232	26.149		51.79
ATOM	4299	0	VAL	758		-16.055	25.258		49.80
MOTA	4300	N	ALA	759	54.622		27.386		54.80
ATOM	4301	CA	ALA	759	54.825		27.814		57.15
ATOM	4302	CB	ALA	759	55.406		29.212		56.77
ATOM	4303	C	ALA	759	53.524		27.777		60.83
ATOM	4304	0	ALA	759	53.487		27.296		63.59
MOTA	4305	N	LEU	760	52.452		28.271	1.00	
ATOM	4306	CA	LEU	760	51.151		28.295	1.00	
MOTA	4307	CB	LEU	760	50.280		29.388	1.00	
MOTA	4308	CG	LEU	760	50.808		30.812	1.00	
ATOM	4309	CD1		760	49.917		31.815	1.00	
ATOM	4310	CD2	LEU	760	50.899		31.138	1.00	

ATO		-	LEU	760	50 4	39 -17.70	36	
ATO		12 0	LEU	760		82 -18.12		00 03,42
ATOM			THR	761				
ATON	1 431	4 CA	THR	761		13 -17.20		
ATOM		.5 CB	THR	761		12 -17.10		
ATOM		6 OG1		761		94 -15.73		2 1.00 68.21
ATOM	431	7 CG2		761	50.13	93 -14.69	5 24.70	1 1.00 70.34
ATOM	431		THR	761		2 -15.68		1.00 64.45
ATOM	431		THR	761		30 -18.22		1.00 69.65
ATOM			CYS	1603	52.23	0 -18.49		1.00 70.43
ATOM			MET	534	18.66			0.50 30.57
ATOM			MET	534	69.41			0.50 36.86
ATOM	432		MET		69.16		9 24.646	0.50 40.20
ATOM	4324	_	CYS	534	70.20		9 25.912	0.50 41.95
ATOM	4325		TIP	603	56.21		2 16.341	
ATOM	4326	_		1	71.8 <i>6</i>		2.719	
ATOM	4327		TIP	2	39.67		15.837	1.00 36.87
ATOM	4328		TIP	3	83.76		10.549	1.00 26.81
ATOM	4329		TIP	4	83.84		7.757	1.00 30.07
ATOM	4330		TIP	5	75.192	2 16.430		1.00 26.76
ATOM	4331		TIP	6	86.579	9 19.662		1.00 36.11
ATOM	4332	_	TIP	7	52.204	10.911		1.00 36.83
ATOM	4332		TIP	8	55.174	9.435		1.00 36.83
ATOM	4334		TIP	9	57.077	4.556	32.580	1.00 21.93
ATOM			TIP	10	52.281	4.737	13.300	1.00 20.79
ATOM	4335		TIP	11	41.402		22.893	
ATOM	4336	OH2		12	45.088		21.604	
ATOM	4337		TIP	13	64.519		28.799	1.00 35.14
ATOM	4338		rip	14	77.327	12.960	23.832	1.00 47.52
ATOM	4339	OH2		15	79.366	17.021	18.247	1.00 34.47
ATOM	4340		rip	16	83.087	11.573	15.986	1.00 47.49
ATOM	4341		rip	17	13.977	-9.804	0.222	1.00 22.80
ATOM	4342	OH2 1		18	38.451	0.155	5.081	1.00 24.88
ATOM	4343	OH2 T		20	27.109	6.286	4.902	1.00 41.03
	4344	OH2 T		21	34.379	-1.750	16.771	1.00 27.69
ATOM	4345		'IP	22	20.394	2.449	27.821	1.00 47.69
ATOM	4346	OH2 T	'IP	23	50.587		38.062	1.00 54.32
ATOM	4347		ΙP	24	17.137	-5.949	-1.716	1.00 45.31
ATOM	4348		IP	25	27.604	7.961	15.119	1.00 27.63
ATOM	4349	OH2 T		26	31.446	0.136	6.605	1.00 47.19
ATOM	4350	OH2 T		27		-13.047		1.00 29.98
ATOM	4351	OH2 T		28	28.477	-17 191		1.00 28.86
ATOM	4352	OH2 T		29	88.748	14.279		1.00 37.44
ATOM	4353	OH2 T		30	-2.392	-3.684		1.00 32.72
ATOM	4354	OH2 T	ΙP	31	34.968	-4.221	11.343	1.00 41.86
ATOM	4355	OH2 T	ΙP	32	80.581	17.982	18.549	1.00 40.51
ATOM	4356	OH2 TI	ſΡ	33	5.522			1.00 27.85
ATOM	4357	OH2 TI		34	-10.747	3.773	10.805	1.00 24.60
MOTA	4358	OH2 TI		35	29.049	5.416		1.00 29.27
ATOM		OH2 TI		36		-8.816		1.00 35.24
ATOM		OH2 TI		37	5.871 31.834	3.463		L.00 26.62
ATOM		OH2 TI	_	38		2.899		L.00 <b>4</b> 9.70
ATOM		OH2 TI		39	19.799		-3.941	1.00 29.67
			_		62.060	2.679	32.659 ]	00 54.86



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MOTA	4363	OH	TIP	40	21.100	-6.883	-4.054	1.00 22.33
MOTA	4364	OH2	TIP	41	-15.675	8.744	22.559	1.00 44.54
ATOM	4365	OH2	? TIP	42	40.066	2.225	8.567	1.00 57.00
ATOM	4366	OH2		43	19.477	11.293	-0.049	1.00 37.77
ATOM	4367	OH2	TIP	44	67.060	9.047	17.334	1.00 25.14
ATOM	4368	OH2		45	87.829	18.937	18.529	1.00 45.92
ATOM	4369	OH2		46	74.741	16.956	3.987	1.00 40.33
ATOM	4370	OH2		47	29.411	16.888	10.525	1.00 38.41
ATOM	4371	OH2		48	66.592	7.020	15.108	1.00 36.15
ATOM	4372	OH2	TIP	49	85.071	21.432	5.755	1.00 19.89
ATOM	4373	OH2	TIP	50	-4.842	3.281	3.118	1.00 28.22
ATOM	4374	OH2		51	19.454	5.250	4.876	1.00 34.86
ATOM	4375	OH2	TIP	53	34.785	5.433	24.743	1.00 30.40
ATOM	4376	OH2		54	34.792	-17.150	13.665	1.00 35.81
ATOM	4377	OH2		55	59.956	7.380	27.941	1.00 36.76
ATOM	4378	OH2		56	-7.327	-1.518	6.428	1.00 39.13
MOTA	4379	OH2		57	55.164	12.120	25.338	1.00 38.87
ATOM	4380	OH2		58	68.637	6.832	16.698	1.00 54.96
ATOM	4381	OH2		59	73.778	20.869	19.031	1.00 35.01
ATOM	4382	OH2		60	3.582	-8.363	-8.103	1.00 16.71
MOTA	4383	OH2		61	38.051	10.933	5.487	1.00 32.85
ATOM	4384	OH2		62	29.727	-9.630	-1.370	1.00 30.92
ATOM	4385	OH2		64	49.186	1.253	12.066	1.00 42.67
ATOM	4386	OH2	TIP	65	41.375	3.989	28.951	1.00 37.95
ATOM	4387	OH2	TIP	66	10.798	-13.119	1.125	1.00 38.26
ATOM	4388	OH2	TIP	67	-1.079	-4.386	21.428	1.00 27.92
ATOM	4389	OH2	TIP	68	30.327	16.346	13.295	1.00 53.21
ATOM	4390	OH2	TIP	69	8.319	4.437	3.449	1.00 23.63
ATOM	4391	OH2	TIP	70	73.152	18.809	22.631	1.00 36.45
ATOM	4392	OH2	TIP	71	-7.984	-3.476	25.048	1.00 33.16
ATOM	4393	OH2	TIP	72	66.529	-4.720	28.421	1.00 66.32
ATOM	4394	OH2	TIP	73		-20.723	4.868	1.00 48.14
ATOM ATOM	4395	OH2	TIP	74	59.417	-6.760	4.957	1.00 48.73
ATOM	4396 4397	OH2	TIP	75		-13.306	-2.942	1.00 41.02
ATOM		OH2	TIP	76	-15.064	7.473	4.275	1.00 26.77
ATOM	4398	OH2	TIP	77	33.118	2.917	13.384	1.00 41.38
ATOM	4399	OH2	TIP TIP	78	0.112	-2.913	10.809	1.00 27.49
ATOM	4400	OH2		79	17.448	2.562	5.507	1.00 16.32
ATOM	4401 4402	OH2	TIP	81 82	27.445	3.796	6.134	1.00 29.83
ATOM	4403				-8.708	6.231	9.598	1.00 27.66
ATOM	4404	OH2		83	1.565	-1.998	8.758	1.00 33.46
ATOM -	4405	OH2		84	-4.774	-3.153	7.049	1.00 36.59
ATOM	4406	OH2		85 86	17.443	3.105	1.795	1.00 20.39
ATOM	4407	OH2		86	20.120	3.387	2.918	1.00 30.35
ATOM	4408	OH2		87	0.466	-2.238	22.190	1.00 20.30
ATOM				88	19.749	-6.018	-1.687	1.00 21.33
ATOM	4409	OH2		89		-15.695	6.861	1.00 38.80
ATOM	4410 4411	OH2 OH2		90 01		-12.113	11.774	1.00 34.18
ATOM				91 92	6.297	1.090	-3.192	1.00 24.40
ATOM	4412 4413	OH2		92 93	-13.540	1.554	5.413	1.00 34.94
ATOM	4413	OH2 OH2		93 94	15.607	-7.315	0.017	1.00 26.30
	3374	Onz	IIB	94	-1.868	-5.461	3.839	1.00 37.12



		415	OH2 T	'IP 95	12 710 -
		416	ОН2 Т		50.040 -4.401 1.00 40.61
AT	_	417	OH2 T		24.784 27.233 2.056 1.00 41.42
AT		418	OH2 T		50.15 0.143 1.00 52.75
ATO	OM 44	119	OH2 T		30.424 -4.582 34.237 1.00 42.02
ATO		120	OH2 T		3.485 1.00 61.53
ATO		121		IP 101	-3.999 4.718 1.00 29 02
ATC		22	OH2 T		73.003 -1.967 10.565 1.00 59 23
ATC			OH2 TI		36.672 5.701 30.623 1.00 30.51
ATC			ОН2 ТІ		0.620 11.780 1.00 53 77
ATO	M 44		ОН2 ТІ		6.462 16.955 1.00 27.62
ATO		26 (	OH2 TI		5.550 0.791 19.345 1.00 77.65
ATO	M 44		OH2 TI		3.000 -8.451 22.197 1.00 49.50
ATO	M 44:		OH2 TI		12.308 8.471 17.441 1 00 31 60
ATO			DH2 TI		20.733 -10.524 -0.894 1.00 25 26
ATO	M 443		H2 TI		2.026 18.156 1.00 35 97
ATO	M 443		H2 TI		-1.822 12.848 3.561 1.00 35 44
OTA	443		H2 TI		33.304 13.491 33.225 1 00 10 15
ATOM	1 443		H2 TIE		4.402 -10.813 1.929 1.00 47 07
MOTA	1 443		H2 TIE		8.032 2.916 0.940 1.00 40 79
ATOM	1 443		H2 TIF		75.905 1.522 25.912 1.00 55 51
ATOM	443		H2 TIP		48.960 15.737 14.249 1 00 38 87
ATOM		_	H2 TIP	_	2.333 -11.271 9.174 1 00 29 12
ATOM	443		H2 TIP		83.062 26.404 12.925 1.00 11.17
ATOM			H2 TIP		8.816 -6.440 -3.424 1.00 48 26
ATOM	444		H2 TIP		-8.594 4.575 4.258 1 00 33 cs
ATOM			12 TIP		7.695 -13.769 B.481 1.00 30 30
ATOM			12 TIP		51.500 6.285 10.369 1 00 25 10
ATOM	4443		2 TIP	122	20.720 3.849 15.625 1.00 22.46
ATOM	4444		2 TIP	123	73.111 3.718 20.617 1.00 28.26
ATOM	4445		2 TIP	124	5.312 -11.608 22.516 1.00 22.51
ATOM	4446			125	34.207 2.437 16.601 1.00 65.04
ATOM	4447		2 TIP	126	9.535 -11.998 7.085 1.00 35 13
ATOM	4448		2 TIP	127	8.227 3.912 -1.495 1.00 42 72
ATOM	4449		2 TIP	129	7.312 7.072 2.922 1.00 47.65
ATOM	4450		2 TIP	130	35.824 -1.660 0.135 1.00.30.43
ATOM	4451		2 TIP	131	44.723 10.285 11.144 1 00 32 74
ATOM	4452		2 TIP	132	27.941 -13.172 18.733 1 00 50 55
ATOM	4453		TIP	133	45.301 11.497 21.408 1 00 35 00
ATOM	4454	OH	TIP	134	57.705 -10.824 14.202 1 00 60 10
ATOM	4455		TIP	135	-3.108 15.385 16 685 1 00 30 65
ATOM	4456		TIP	136	85.884 11.182 9.044 1.00.32 04
ATOM	4457			137	12.840 -2.444 1 983 1 00 30 00
ATOM	4458		TIP	138	75.645 3.496 20.607 1.00 33.04
ATOM	4459		TIP	139	13.020 7.518 -2.510 1.00 40 60
ATOM	4460		TIP	140	11 245 10 000
ATOM			TIP	141	50 563 70 000
ATOM	4461		TIP	142	13 671 76 71 76 71 34
ATOM	4462		TIP	143	-6 350
ATOM	4463		TIP	144	25 620 12 77 1.00 37.08
ATOM	4464		TIP	145	-16 450 30 31
ATOM	4465		TIP	146	96 500 70 70 70 70 70 70 70 70 70 70 70 70 7
Ori	4466	OH2	TIP	147	32 130 47.80
					32.139 ~4.674 1.757 1.00 32.43

ATOM	4467	OH2	TIP	148	44.890	7.505	11.806	1.00 32.46
MOTA	4468	OH2	TIP	149	80.781	12.432	16.562	1.00 47.77
ATOM	4469	OH2	TIP	150	3.017	-7.101	-1.917	1.00 40.92
MOTA	4470	OH2	TIP	151	31.784	-6.139	20.968	1.00 38.23
MOTA	4471	OH2	TIP	152	74.835	-2.597	12.290	1.00 48.89
ATOM	4472	OH2	TIP	153	7.509	6.768	-1.083	1.00 46.02
MOTA	4473	OH2	TIP	154	71.732	5.360	21.908	1.00 33.30
ATOM	4474	ОН2	TIP	155	68.150	-5.075	8.794	1.00 39.31
ATOM	4475	OH2	TIP	156	0.148	-9.544	6.872	1.00 41.37
ATOM	4476	OH2	TIP	157	67.878	18.204	10.861	1.00 51.19
ATOM	4477	OH2	TIP	158	3.652	8.829	4.428	1.00 31.24
ATOM	4478	OH2	TIP	159	52.100	11.362	18.433	1.00 40.73
MOTA	4479	ОН2		161	-10.357	6.783	4.861	1.00 35.13
ATOM	4480	OH2	TIP	162	76.471	1.562	-0.853	1.00 59.17
ATOM	4481	OH2	TIP	163	10.073	-12.056	17.071	1.00 44.69
ATOM	4482	OH2	TIP	164	34.163	14.271	18.254	1.00 39.59
ATOM	4483	OH2		165	2.320	-7.990	16.820	1.00 38.19
ATOM	4484	OH2		166	29.696	1.908	6.098	1.00 38.02
ATOM	4485	OH2		167		-17.410	11.766	1.00 48.15
ATOM	4486	OH2		168	42.244	18.049	11.043	1.00 50.95
ATOM	4487	OH2		169	87.907	10.574	5.721	1.00 50.33
ATOM	4488	OH2		170	70.313	3.998	25.141	1.00 80.28
MOTA	4489	OH2		171	77.603	5.679	23.952	1.00 43.23
ATOM	4490	OH2	TIP	172	-0.942	-8.153	4.508	1.00 43.23
ATOM	4491	OH2	TIP	173	34.297	15.574	1.690	1.00 33.10
ATOM	4492	OH2	TIP	174	-9.643	7.829	7.414	1.00 50.48
MOTA	4493	OH2	TIP	175	11.618	5.655	7.455	
ATOM	4494	OH2	TIP	176	-8.705	13.841	13.642	1.00 43.37
ATOM	4495	OH2	TIP	177	32.009	3.416	18.257	1.00 72.49
ATOM	4496	OH2	TIP	178	-8.651	10.180	24.352	1.00 44.16
ATOM	4497	OH2	TIP	179	-1.153	-6.532	15.548	1.00 44.85
ATOM	4498	OH2	TIP	180	80.235	0.749	15.548	1.00 32.90
ATOM	4499	OH2	TIP	181	67.222	20.490	-1.574	1.00 34.75
ATOM	4500	OH2	TIP	182	-0.471	4.367	1.248	1.00 40.76
MOTA	4501	OH2	TIP	183	0.149	6.517	2.578	1.00 36.58
ATOM	4502	OH2	TIP	184	-1.186	8.867		1.00 40.12
ATOM	4503	OH2	TIP	185	-5.093	9.260	1.311	1.00 44.77
ATOM	4504	OH2	TIP	186	-7.235		2.252	1.00 52.07
ATOM	4505	OH2	TIP	187	2.724	10.227	3.913	1.00 58.53
ATOM	4506		TIP	188		7.169 11.031	0.879	1.00 47.77
ATOM	4507		TIP	189	5.527 63.927		8.519	1.00 34.40
ATOM	4508		TIP	190	79.264	12.721	22.689	1.00 40.75
MOTA	4509	OH2		191		1.066	18.321	1.00 41.34
ATOM	4510	OH2		192		-11.825 -0.972	7.256	1.00 79.86
ATOM	4511	OH2			13.994		-4.310	1.00 31.15
ATOM	4512	OH2		193	59.546	3.024	33.227	1.00 40.34
MOTA	4512			194	32.179	13.637	19.964	1.00 48.25
ATOM		OH2		195	72.178	16.188	22.879	1.00 42.72
	4514	OH2		196	0.898	-8.663	14.348	1.00 41.76
ATOM	4515	OH2		197	-0.490	5.455	30.574	1.00 38.30
ATOM	4516	OH2		199	-1.277	-4.244	27.691	1.00 56.27
ATOM	4517	OH2		200	81.605	15.360	17.272	1.00 42.05
ATOM	4518	OH2	TIP	201	-17.534	4.081	23.779	1.00 59.65
					•			

<b>አ</b> ጥር	NA			
ATC ATC				27.748 10.634 14.595 1.00 49 97
ATO				34 991 4 450
				-3 460
ATO		<b>-</b> .	IP 205	42 705 2 500
ATO				52 902 11 050
ATO				26 971 14 25 1.00 35.12
ATO		5 OH2 T	P 208	-7 104
ATO		6 OH2 TI		96 676 5 7-1
OTA			P 210	55 000 15 000
OTA	M 452	8 OH2 TI		1.00 68.75
ATON				10 000
ATOM	453			19.988 7.127 6.976 1.00 45.55
ATOM	453			28.905 2.021 -3.430 1.00 48.55
ATOM	1 4532	OH2 TI		26.446 2.593 -4.753 1.00 55.04
ATOM				36.539 2.911 18.446 1.00 30 50
ATOM			·	10.807 -20.725 14.119 1 00 56 02
ATOM				28.203 -14.485 6.172 1.00 62.00
ATOM				31.519 1.503 -2.010 1 00 56 10
ATOM				10.014 -16.571 15.451 1 00 46 27
ATOM	4538			7.126 -11.922 5.526 1.00 56.00
ATOM				-12.414 14.643 10.965 1.00 67.36
ATOM			- <del>-</del>	10 979 0 733
ATOM				11 202 10 30.81
ATOM	_			24 011 10 1-1
ATOM	4542			31 105 17 22
ATOM	4543			36 057 77 77 77 77 77 77 77 77 77 77 77 77 7
	4544	OH2 TIP	227	35 170 3 171 3.00 50,98
ATOM	4545	OH2 TIP		64 027 12 225
ATOM	4546	OH2 TIP	229	36 514 6 15-
ATOM	4547	OH2 TIP	230	90 607
ATOM	4548	OH2 TIP	231	49 907 11 07-
ATOM	4549	OH2 TIP	232	60 200 70 70
ATOM	4550	OH2 TIP	233	10 154 27 25
ATOM	4551	OH2 TIP	234	66 100 33.60
ATOM	4552	OH2 TIP	235	75 153 10 25 1.00 56.92
ATOM	4553	OH2 TIP	236	-3 885 10 34.22
ATOM	4554	OH2 TIP	237	5 034
ATOM	4555	OH2 TIP	238	35 910 6 160
ATOM	4556	OH2 TIP	239	E 404 16 50-
MOTA	4557	OH2 TIP	240	15 333 1.00 65.17
ATOM	4558	OH2 TIP	241	46.332 -11.698 26.865 1.00 55.30
MOTA	4559	OH2 TIP	242	6.179 6.434 13.895 1.00 45.92
ATOM	4560	OH2 TIP	243	-3.869 -4.958 20.821 1.00 41.96
ATOM	4561	OH2 TIP	244	1.690 -3.598 -0.200 1.00 41.42
ATOM	4562	OH2 TIP		00.181 11.454 23.000 1 00 56 22
ATOM	4563	OH2 TIP	245	10.501 7.621 5.627 1.00 77 40
ATOM	4564	OH2 TIP	246	3.007 8.485 2.181 1.00 89.31
ATOM	4565	OH2 TIP	247	64.552 -8.093 20.595 1.00 45 96
ATOM	4566	OH2 TIP	248	11.243 -17.828 13.332 1.00 65 30
ATOM			249	42.226 -6.785 14.857 1.00 81.78
ATOM		OH2 TIP	250	2.875 -4.176 22.032 1.00 53.45
ATOM		OH2 TIP	251	72.048 1.134 -2.037 1.00 38.85
ATOM		OH2 TIP	252	EA 358
ALON	4570	OH2 TIP	254	E7 772
				37.772 9.500 11.808 1.00 40.03



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MOTA	4571	OH2		255	43.306	20.459	30.366	1.00	47.59
MOTA	4572	OH2		256	67.064	16.514	15.765	1.00	57.51
ATOM	4573	OH2	TIP	257	87.612	21.648	5.147	1.00	70.52
MOTA	4574	OH2	TIP	258	21.095	9.853	-9.308	1.00	78.97
MOTA	4575	OH2	TIP	261	71.914	28.544	7.912	1.00	83.90
MOTA	4576	OH2	TIP	262	25.727	-8.133	27.190	1.00	54.87
ATOM	4577	OH2	TIP	263	-18.738	10.877	12.767	1.00	71.80
MOTA	4578	OH2	TIP	264	30.524	11.543	16.329	1.00	46.98
MOTA	4579	OH2	TIP	265	22.211	-16.242	-2.763	1.00	55.17
MOTA	4580	OH2	TIP	266	29.755	9.037	18.396	1.00	67.93
ATOM	4581	C1	MON	1000	67.458	4.500	11.935	1.00	0.00
ATOM	4582	C2	MON	1000	67.015	3.958	10.687	1.00	0.00
ATOM	4583	ΝЗ	МОИ	1000	67.367	2.732	10.160	1.00	0.00
ATOM	4584	C4	MON	1000	66.127	4.618	9.793	1.00	0.00
ATOM	4585	C5	MON	1000	65.620	5.919	10.125	1.00	0.00
ATOM	4586	C6	MON	1000	66.041	6.508	11.380	1.00	0.00
ATOM	4587	C7	MON	1000	66.948	5.809	12.276	1.00	0.00
ATOM	4588	C8	MON	1000	65.933	3.759	8.668	1.00	0.00
ATOM	4589	C10	MON	1000	66.745	2.518	8.922	1.00	0.00
MOTA	4590	C11	MON	1000	65.043	4.051	7.483	1.00	0.00
ATOM	4591	012	MON	1000	66.862	1.516	8.241	1.00	0.00
ATOM	4592	C13	MON	1000	64.479	2.990	6.570	1.00	0.00
ATOM	4593	C14	MON	1000	63.459	3.330	5.617	1.00	0.00
ATOM	4594	C15	MON	1000	62.923	2.333	4.727	1.00	0.00
ATOM	4595	C16	MON	1000	63.379	0.956	4.754	1.00	0.00
ATOM	4596	C17	MON	1000	64.960	1.637	6.605	1.00	0.00
ATOM	4597		MON	1000	64.418	0.642	5.713	1.00	0.00
ATOM	4598		MON	1000	62.848	-0.025	3.880	1.00	0.00
ATOM	4599	C20		1000	63.429	-1.407	3.816	1.00	0.00
ATOM	4600		MON	1000	61.888	0.343	2.786	1.00	0.00
ATOM	4601	C22		1000	61.085	-0.818	2.152	1.00	0.00
ATOM	4602	N23		1000	61.868	-2.035	1.930	1.00	0.00
ATOM	4603		MON	1000	62.562	-2.492	3.133	1.00	0.00
ATOM	4604		MON	1000	61.481	-2.328	-0.389	1.00	0.00
ATOM	4605		MON	1000	62.001	-2.670	0.659	1.00	0.00
ATOM	4606	Cl	MON	1001	5.458	3.340	18.422	1.00	0.00
ATOM	4607	C2	MON	1001	6.049	3.475	19.718	1.00	0.00
ATOM	4608	N3	MON	1001	5.935	2.580	20.763	1.00	0.00
ATOM	4609	C4	MON	1001	6.857	4.573	20.124	1.00	0.00
ATOM	4610	C5	MON	1001	7.121	5.641	19.202	1.00	0.00
ATOM	4611	C6	MON	1001	6.543	5.548	17.877	1.00	0.00
ATOM	4612	C7	MON	1001	5.722		17.489	1.00	0.00
MOTA	4613	C8	MON	1001	7.250	4.340	21.477	1.00	0.00
ATOM	4614		MON	1001	6.647	3.023	21.886	1.00	0.00
ATOM	4615		MON	1001	8.138	5.242	22.302	1.00	
ATOM	4616	012		1001	6.735	2.426	22.943		0.00
ATOM	4617		MON	1001	8.918	4.783		1.00	0.00
ATOM	4618	C14		1001	9.913		23.509	1.00	0.00
ATOM	4619	C15				5.641	24.091	1.00	0.00
ATOM	4620	C16		1001	10.654	5.224	25.253	1.00	0.00
				1001	10.435	3.935	25.881	1.00	0.00
ATOM ATOM	4621	C17		1001	8.670	3.508	24.123	1.00	0.00
AI ON	4622	C18	HOIN	1001	9.416	3.095	25.285	1.00	0.00

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ATOM ATOM ATOM ATOM ATOM ATOM ATOM	4623 4624 4625 4626 4627 4628 4629	N19 MON C20 MON C21 MON C22 MON N23 MON C24 MON O25 MON	1001 1001 1001 1001 1001 1001	11.168 10.831 12.107 13.125 12.570 11.902 13.118	3.525 2.255 4.463 3.821 2.742 1.711	27.023 27.749 27.725 28.698 29.518 28.725	1.00 1.00 1.00 1.00 1.00	0.00 0.00 0.00 0.00 0.00
ATOM	4629	C26 MON	1001 1001	13.118 12.610	3.569 2.731	31.669	1.00	0.00

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### CLAIMS

What is claimed is:

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1. A crystalline form of a polypeptide corresponding to the catalytic domain of a protein tyrosine kinase.

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2. The crystalline form of claim 1, wherein said protein tyrosine kinase is a receptor protein tyrosine kinase.

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3. The crystalline form of claim 2, wherein said receptor protein tyrosine kinase is selected from the group consisting of PDGF-R, FLK, CCK4, MET, TRKA, AXL, TIE, EPH, RYK, DDR, ROS, RET, LTK, ROR1, and MUSK.

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4. The crystalline form of claim 1, wherein said protein tyrosine kinase is a non-receptor protein tyrosine kinase.

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5. The crystalline form of claim 4, wherein said non-receptor protein tyrosine kinase is selected from a group consisting of SRC, BRK, BTK, CSK, ABL, ZAP70, FES, FAK, JAK, and ACK.

6. The crystalline form of claim 1, comprising one or more heavy metal atoms.

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7. The crystalline form of claim 1, wherein said

protein tyrosine kinase is FGFR.

8. The crystalline form of claim 7, wherein said FGFR is FGFR1.

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- 9. The crystalline form of claim 8, defined by atomic structural coordinates set forth in Table 1.
- 10. The crystalline form of claim 7, comprising at least one compound.
  - 11. The crystalline form of claim 10, wherein said compound is a nucleotide analog.

12. The crystalline form of claim 11, wherein said nucleotide analog is AMP-PCP.

13. The crystalline form of claim 12, defined by atomic structural coordinates set forth in Table 2.

- 14. The crystalline form of claim 10, wherein said compound is an indolinone compound.
- 15. The crystalline form of claim 14, wherein said indolinone compound has a structure set forth in formula I or II:

$$R_{5}$$

$$R_{6}$$

$$R_{6}$$

$$R_{7}$$

$$R_{1}$$

$$R_{4}$$

$$CR_{3}$$

$$R_{6}$$

$$R_{6}$$

$$R_{6}$$

$$R_{7}$$

$$R_{1}$$

$$R_{1}$$

$$R_{2}$$

$$R_{1}$$

$$R_{2}$$

$$R_{1}$$

$$R_{2}$$

$$R_{1}$$

$$R_{2}$$

$$R_{3}$$

$$R_{4}$$

$$R_{5}$$

$$R_{6}$$

$$R_{7}$$

$$R_{1}$$

$$R_{1}$$

$$R_{2}$$

$$R_{3}$$

$$R_{4}$$

$$R_{5}$$

$$R_{6}$$

$$R_{7}$$

$$R_{1}$$

$$R_{1}$$

$$R_{2}$$

$$R_{3}$$

$$R_{4}$$

$$R_{5}$$

$$R_{6}$$

$$R_{7}$$

$$R_{1}$$

$$R_{1}$$

$$R_{2}$$

$$R_5$$
 $A_2$ 
 $A_1$ 
 $R_6$ 
 $A_3$ 
 $A_4$ 
 $R_7$ 
 $R_1$ 
 $R_1$ 
 $R_1$ 
 $R_1$ 
 $R_1$ 
 $R_2$ 

or a pharmaceutically acceptable salt, isomer, metabolite, ester, amide, or prodrug thereof, wherein

- (a)  $A_1$ ,  $A_2$ ,  $A_3$ , and  $A_4$  are independently carbon or nitrogen;
  - (b) R<sub>1</sub> is hydrogen or alkyl;
- (c)  $R_2$  is oxygen in the case of an oxindolinone or sulfur in the case of a thiolindolinone;
  - (d) R<sub>3</sub> is hydrogen;
    - (e)  $R_4$ ,  $R_5$ ,  $R_6$ , and  $R_7$  are optionally present and are

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either (i) independently selected from the group consisting of hydrogen, alkyl, alkoxy, aryl, aryloxy, alkaryl, alkaryloxy, halogen, trihalomethyl, S(0)R,  $SO_2NRR'$ ,  $SO_3R$ , SR,  $NO_2$ , NRR', OH, CN, C(O)R, OC(O)R, NHC(O)R,  $(CH_2)_nCO_2R$ , and CONRR' or (ii) any two adjacent  $R_4$ ,  $R_5$ ,  $R_6$ , and  $R_7$  taken together form a fused ring with the aryl portion of the oxindole-based portion of the indolinone;

- (f) R<sub>2</sub>', R<sub>3</sub>', R<sub>4</sub>', R<sub>5</sub>', and R<sub>6</sub>' are each independently selected from the group consisting of hydrogen, alkyl, alkoxy, aryl, aryloxy, alkaryl, alkaryloxy, halogen, trihalomethyl, S(O)R, SO<sub>2</sub>NRR', SO<sub>3</sub>R, SR, NO<sub>2</sub>, NRR', OH, CN, C(O)R, OC(O)R, NHC(O)R, (CH<sub>2</sub>)<sub>n</sub>CO<sub>2</sub>R, and CONRR';
- 15 (g) n is 0, 1, 2, or 3;
  - (h) R is hydrogen, alkyl or aryl;
  - (i) R' is hydrogen, alkyl or aryl; and
- (j) A is a five membered heteroaryl ring selected from the group consisting of thiophene, pyrrole, 20 pyrazole, imidazole, 1,2,3-triazole, 1,2,4-triazole, oxazole, isoxazole, thiazole, isothiazole, furan, 1,2,3oxadiazole, 1,2,4-oxadiazole, 1,2,5-oxadiazole, 1,3,4oxadiazole, 1,2,3,4-oxatriazole, 1,2,3,5-oxatriazole, 1,2,3-thiadiazole, 1,2,4-thiadiazole, 1,2,5-thiadiazole, 25 1,3,4-thiadiazole, 1,2,3,4-thiatriazole, 1,2,3,5thiatriazole, and tetrazole, optionally substituted at one or more positions with alkyl, alkoxy, aryl, aryloxy, alkaryl, alkaryloxy, halogen, trihalomethyl, S(O)R,  $SO_2NRR'$ ,  $SO_3R$ , SR,  $NO_2$ , NRR', OH, CN, C(O)R, OC(O)R, 30 NHC(O)R,  $(CH_2)_nCO_2R$  or CONRR'.



- 16. The crystalline form of claim 15, wherein said indolinone compound is 3-[(3-(2-carboxyethyl)-4-methylpyrrol-5-yl)methylene]-2-indolinone.
- 5 17. The crystalline form of claim 15, wherein said indolinone compound is 3-[4-(4-formylpiperazine-1-yl)benzylidenyl]-2-indolinone.
  - 18. The crystalline form of claim 16, defined by the atomic structural coordinates of Table 3.
    - 19. The crystalline form of claim 17, defined by the atomic structural coordinates of Table 4.
    - 20. The crystalline form of claim 1, having monoclinic unit cells.
      - 21. The crystalline form of claim 20, wherein said monoclinic unit cells have dimensions of about a=208.3 Å, b=57.8 Å, c=65.5 Å and  $\beta$ =107.2°.
      - 22. The crystalline form of claim 20, wherein said monoclinic unit cells have dimensions of about a=211.6 Å, b=51.3 Å, c=66.1 Å and  $\beta$ =107.7°.
      - 23. The crystalline form of claim 10, comprising one or more heavy metal atoms.
- 24. A polypeptide corresponding to the catalytic

  domain of a protein tyrosine kinase, containing at least
  about 20 amino acid residues upstream of the first

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glycine in the conserved glycine-rich region of the catalytic domain, and at least about 17 amino acid residues downstream of the conserved arginine located at the C-terminal boundary of the catalytic domain.

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25. The polypeptide of claim 24, wherein said protein tyrosine kinase is a receptor protein tyrosine kinase.

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26. The polypeptide of claim 24, wherein said protein tyrosine kinase is a non-receptor protein tyrosine kinase.

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27. The polypeptide of claim 25, wherein said receptor tyrosine kinase is selected from the group consisting of FGF-R, PDGF-R, KDR, CCK4, MET, TRKA, AXL, TIE, EPH, RYK, DDR, ROS, RET, LTK, ROR1, and MUSK.

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28. The polypeptide of claim 26, wherein said non-receptor kinase is selected from the group consisting of SRC, BRK, BTK, CSK, ABL, ZAP70, FES, FAK, JAK, and ACK.

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29. The polypeptide of claim 24 having the amino acid sequence shown in SEQ ID NO:4.

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- 30. A method of using the polypeptide of claim 24 to form a crystal, comprising the steps of:
- (a) mixing a volume of polypeptide solution with a reservoir solution; and

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(b) incubating the mixture obtained in step(a) over the reservoir solution in a closed container,

under conditions suitable for crystallization.

- 31. A method of obtaining an FGF receptor tyrosine kinase domain polypeptide in crystalline form, comprising the steps of:
- (a) mixing a volume of polypeptide solution with an equal volume of reservoir solution, wherein said polypeptide solution comprises 1 mg/mL to 60 mg/mL FGF-type tyrosine kinase domain protein, 10 mM to 200 mM buffering agent, 0 mM to 20 mM dithiothreitol and has a pH of about 5.5 to about 7.5, and wherein said reservoir solution comprises 10% to 30% (w/v) polyethylene glycol, 0.1 M to 0.5 M ammonium sulfate, 0% to 20% (w/v) ethylene glycol or glycerol, 10 mM to 200 mM buffering agent and has a pH of about 5.5 to about 7.5; and
- (a) over said reservoir solution in a closed container at a temperature between 0° and 25° °C until crystals form.

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32. The method of claim 31, wherein said polypeptide solution comprises about 10 mg/mL FGF receptor tyrosine kinase domain, about 10 mM sodium chloride, about 2 mM dithiothreitol, about 10 mM Tris-HCl and has a pH of about 8; the reservoir buffer comprises about 16% (w/v) polyethylene glycol (MW 10000), about 0.3 M ammonium sulfate, about 5% ethylene glycol or glycerol, about 100 mM bis-Tris and has a pH of about 6.5; and the temperature is about 4°C.

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33. The method of claim 31, wherein said

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polypeptide solution comprises a compound.

- 34. A cDNA encoding an FGF receptor tyrosine kinase domain protein, wherein a coding strand of the cDNA has the nucleotide sequence of SEQ ID NO:5.
- 35. A method of determining three dimensional structures of protein tyrosine kinases with unknown structure comprising the step of applying structural atomic coordinates set forth in Table 1, Table 2, Table 3, or Table 4.
- 36. The method of claim 35, comprising the following steps:
- (a) aligning a first computer representation of an amino acid sequence of a protein tyrosine kinase of unknown structure with a second computer representation of a protein tyrosine kinase of known structure by matching homologous regions of amino acid sequences of said first computer representation and said second computer representation;
- (b) transferring computer representations of amino acid structures in said protein tyrosine kinase of known structure to computer representations of corresponding amino acid structures in said protein tyrosine kinase with unknown structure; and
- (c) determining a low energy conformation of the protein tyrosine kinase structure resulting from step (b).
  - 37. The method of claim 35, comprising the

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following steps:

- (a) aligning the positions of atoms in the unit cell by matching electron diffraction data from two crystals; and
- (b) determining a low energy conformation of the resulting protein tyrosine kinase structure.
- 38. The method of claim 35, comprising the following steps:
- (a) determining the secondary structure of a protein tyrosine kinase structure using NMR data; and
- (b) simplifying the assignment of throughspace interactions of amino acids.
- 39. The method of any one of claims 35, 36, 37, or 38, wherein said protein tyrosine kinase with or without known structure is a receptor protein tyrosine kinase.
  - 40. The method of claim 39, wherein said receptor protein tyrosine kinase with or without known structure is selected from the group consisting of FGF-R, PDGF-R, FLK, CCK4, MET, TRKA, AXL, TIE, EPH, RYK, DDR, ROS, RET, LTK, ROR1, and MUSK.
- 41. The method of anyone of claims 35, 36, 37, or 38, wherein said protein tyrosine kinase with or without known structure is a non-receptor protein tyrosine kinase.
- 42. The method of claim 41, wherein said protein tyrosine kinase with or without known structure is

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selected from the group consisting of SRC, BRK, BTK, CSK, ABL, ZAP70, FES, FAK, JAK, and ACK.

- 43. A method of identifying a potential modulator of protein tyrosine kinase function by docking a computer representation of a structure of a compound with a computer representation of a structure of a cavity formed by the active-site of a protein tyrosine kinase, wherein said structure of said protein tyrosine kinase is defined by atomic structural coordinates set forth in Table 1, Table 2, Table 3, or Table 4.
- 44. The method of claim 43, comprising the following steps:
- (a) removing a computer representation of a compound complexed with a protein tyrosine kinase and docking a computer representation of a compound from a computer data base with a computer representation of the active-site of the protein tyrosine kinase;
- (b) determining a conformation of the complex resulting from step (a) with a favorable geometric fit and favorable complementary interactions; and
- (c) identifying compounds that best fit said active-site as potential modulators of protein tyrosine kinase function.
- 45. The method of claim 43, comprising the following steps:
- (a) modifying a computer representation of

  compound complexed with a protein tyrosine kinase by the

  deletion of a chemical group or groups or by the

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addition of a chemical group or groups;

- (b) determining a conformation of the complex resulting from step (a) with a favorable geometric fit and favorable complementary interactions; and
- (c) identifying compounds that best fit the protein tyrosine kinase active-site as potential modulators of protein tyrosine kinase function.
- 46. The method of claim 43, wherein said method comprises the following steps:
- (a) removing a computer representation of a compound complexed with a protein tyrosine kinase; and
- (b) searching a data base for data base compounds similar to said compounds using a compound searching computer program or replacing portions of said compound with similar chemical structures from a data base using a compound construction computer program.
- 47. The method of any one of claims 43, 44, 45, or 46, wherein said protein tyrosine kinase is a receptor protein tyrosine kinase.
  - 48. The method of claim 47, wherein said receptor protein tyrosine kinase is selected from the group consisting of FGF-R, PDGF-R, FLK, CCK4, MET, TRKA, AXL, TIE, EPH, RYK, DDR, ROS, RET, LTK, ROR1, and MUSK.
  - 49. The method of anyone of claims 43, 44, 45, or 46, wherein said protein tyrosine kinase is a non-receptor protein tyrosine kinase.

- 50. The method of claim 49, wherein said protein tyrosine kinase is selected from the group consisting of SRC, BRK, BTK, CSK, ABL, ZAP70, FES, FAK, JAK, and ACK.
- 5 51. a potential modulator of protein tyrosine kinase function identified by the method of any one of claims 43, 44, 45, or 46.
  - 52. The potential modulator of claim 51, wherein said modulator is selected from a computer data base.
  - 53. The potential modulator of claim 51, wherein said modulator is constructed from chemical groups selected from a computer data base.
  - 54. The potential modulator of protein tyrosine kinase function of claim 51, wherein said modulator is an indolinone compound of formula I or II:

$$R_{5}$$

$$R_{6}$$

$$R_{7}$$

$$R_{1}$$

$$R_{6}$$

$$R_{7}$$

$$R_{1}$$

$$R_{4}$$

$$R_{6}$$

$$R_{6}$$

$$R_{6}$$

$$R_{7}$$

$$R_{1}$$

$$R_{1}$$

$$R_{1}$$

$$R_{1}$$

$$R_{2}$$

$$R_{1}$$

$$R_{2}$$

$$R_{1}$$

$$R_{2}$$

$$R_{3}$$

$$R_{6}$$

$$R_{6}$$

$$R_{7}$$

$$R_{1}$$

$$R_{1}$$

$$R_{2}$$

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$$R_5$$
 $A_2$ 
 $A_1$ 
 $R_6$ 
 $A_3$ 
 $A_4$ 
 $R_7$ 
 $R_1$ 
 $R_1$ 
 $R_1$ 
 $R_1$ 
 $R_2$ 

or a pharmaceutically acceptable salt, isomer, metabolite, ester, amide, or prodrug thereof, wherein

- (a)  $A_1$ ,  $A_2$ ,  $A_3$ , and  $A_4$  are independently carbon or nitrogen;
  - (b) R<sub>1</sub> is hydrogen or alkyl;
- (c)  $R_2$  is oxygen in the case of an oxindolinone or sulfur in the case of a thiolindolinone;
  - (d) R<sub>3</sub> is hydrogen;

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- (e)  $R_4$ ,  $R_5$ ,  $R_6$ , and  $R_7$  are optionally present and are either (i) independently selected from the group consisting of hydrogen, alkyl, alkoxy, aryl, aryloxy, alkaryl, alkaryloxy, halogen, trihalomethyl, S(0)R,  $SO_2NRR'$ ,  $SO_3R$ , SR,  $NO_2$ , NRR', OH, CN, C(0)R, OC(0)R, NHC(0)R,  $(CH_2)_nCO_2R$ , and CONRR' or (ii) any two adjacent  $R_4$ ,  $R_5$ ,  $R_6$ , and  $R_7$  taken together form a fused ring with the aryl portion of the oxindole-based portion of the indolinone;
- 20
- (f) R<sub>2</sub>', R<sub>3</sub>', R<sub>4</sub>', R<sub>5</sub>', and R<sub>6</sub>' are each independently selected from the group consisting of hydrogen, alkyl, alkoxy, aryl, aryloxy, alkaryl, alkaryloxy, halogen, trihalomethyl, S(O)R, SO<sub>2</sub>NRR', SO<sub>3</sub>R,

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SR, NO<sub>2</sub>, NRR', OH, CN, C(O)R, OC(O)R, NHC(O)R,  $(CH_2)_nCO_2R$ , and CONRR';

- (g) n is 0, 1, 2, or 3;
- (h) R is hydrogen, alkyl or aryl;
- (i) R' is hydrogen, alkyl or aryl; and
- (j) A is a five membered heteroaryl ring selected from the group consisting of thiophene, pyrrole, pyrazole, imidazole, 1,2,3-triazole, 1,2,4-triazole, oxazole, isoxazole, thiazole, isothiazole, furan, 1,2,3-oxadiazole, 1,2,4-oxadiazole, 1,2,5-oxadiazole, 1,3,4-oxadiazole, 1,2,3,4-oxatriazole, 1,2,3,5-oxatriazole, 1,2,3-thiadiazole, 1,2,4-thiadiazole, 1,2,5-thiadiazole, 1,3,4-thiadiazole, 1,2,3,4-thiatriazole, 1,2,3,5-thiatriazole, and tetrazole, optionally substituted at one or more positions with alkyl, alkoxy, aryl, aryloxy, alkaryl, alkaryloxy, halogen, trihalomethyl, S(O)R, SO<sub>2</sub>NRR', SO<sub>3</sub>R, SR, NO<sub>2</sub>, NRR', OH, CN, C(O)R, OC(O)R, NHC(O)R, (CH<sub>2</sub>)<sub>n</sub>CO<sub>2</sub>R or CONRR'.
- 55. A method of identifying a potential modulator of protein tyrosine kinase function as a modulator of protein tyrosine kinase function, comprising the following steps:
  - (a) administering said potential modulator to cells;
  - (b) comparing the level of protein tyrosine kinase phosphorylation between cells not administered the potential modulator and cells administered said potential modulator; and
- (c) identifying said potential modulator as a modulator of protein tyrosine kinase function based on

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the difference in the level of protein tyrosine kinase phosphorylation.

- 56. A method of identifying a potential modulator of protein tyrosine kinase function as a modulator of protein tyrosine kinase function, wherein said method comprises the following steps:
- (a) administering a preparation of said potential modulator to cells;
- (b) comparing the rate of cell growth between cells not administered the modulator and cells administered the modulator; and
- (c) identifying said potential modulator as a modulator of protein tyrosine kinase function based on the difference in the rate of cell growth.
- 57. A method of treating a disease associated with a protein tyrosine kinase with inappropriate activity in a cellular organism, wherein said method comprises the steps of:
- (a) administering a modulator of protein tyrosine kinase function to the organism, wherein said modulator is in an acceptable pharmaceutical preparation; and
- (b) activating or inhibiting the protein tyrosine kinase function to treat the disease.
- 58. The method of any one of claims 55, 56, or 57, wherein said protein tyrosine kinase is a receptor protein tyrosine kinase.

59. The method of claim 58, wherein said receptor protein tyrosine kinase is selected from the group containing FGF-R, PDGF-R, FLK, CCK4, MET, TRKA, AXL, TIE, EPH, RYK, DDR, ROS, RET, LTK, ROR1, and MUSK.

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60. The method of any one of claims 55, 56, or 57, wherein said protein tyrosine kinase is a non-receptor protein tyrosine kinase.

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61. The method of claim 60, wherein said non-receptor protein tyrosine kinase is selected from a group consisting of SRC, BRK, BTK, CSK, ABL, ZAP70, FES, FAK, JAK, and ACK.

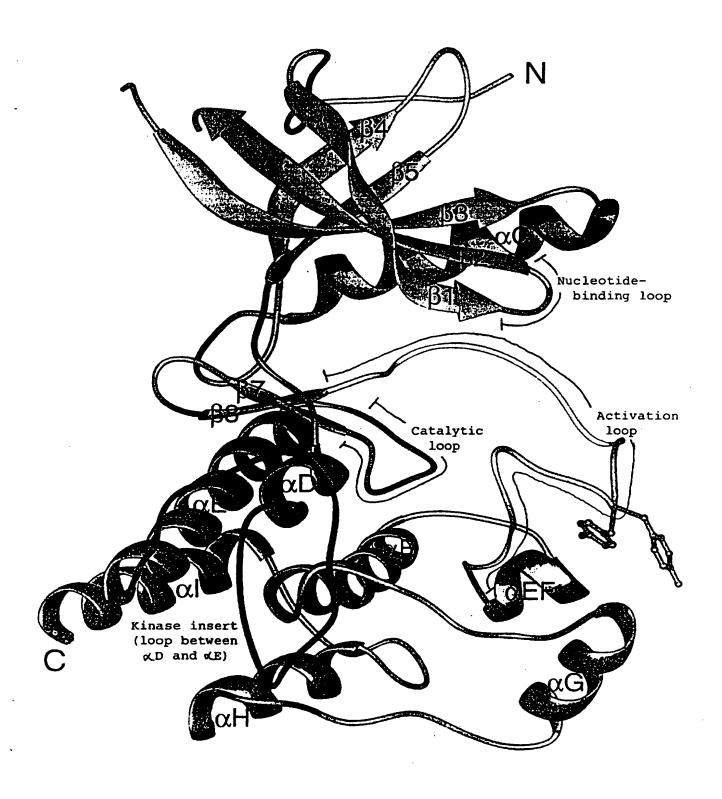
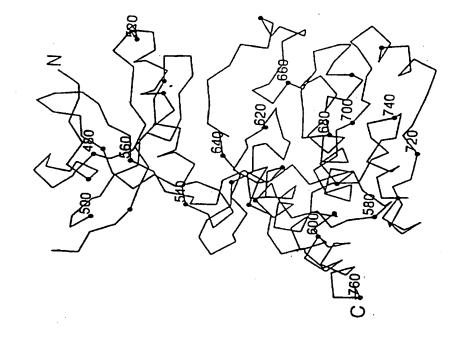


FIGURE 1





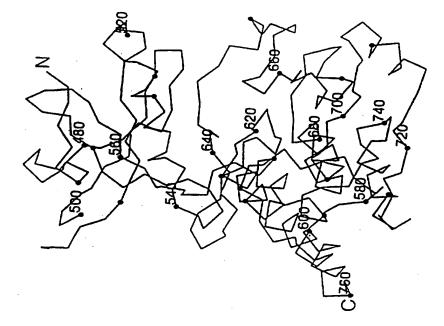


FIGURE 2



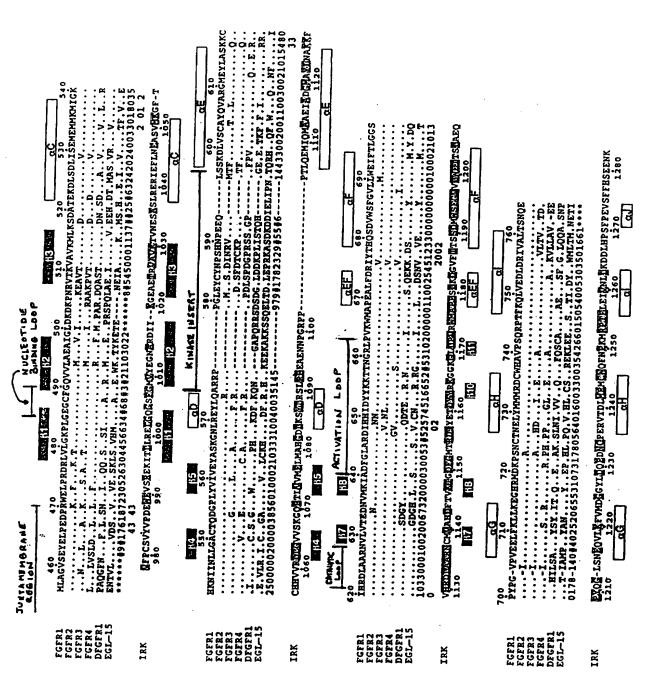
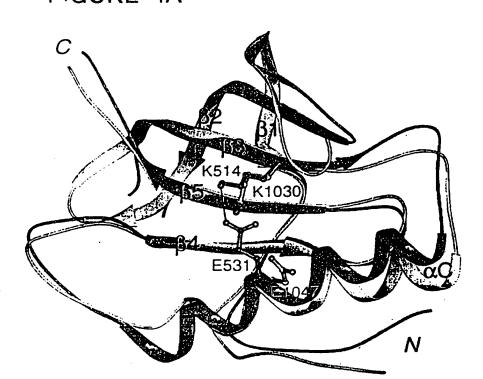
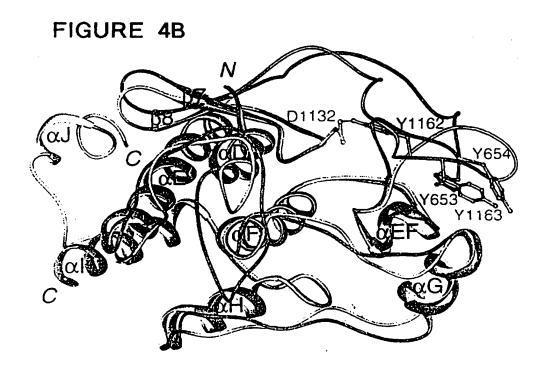


FIGURE 4A



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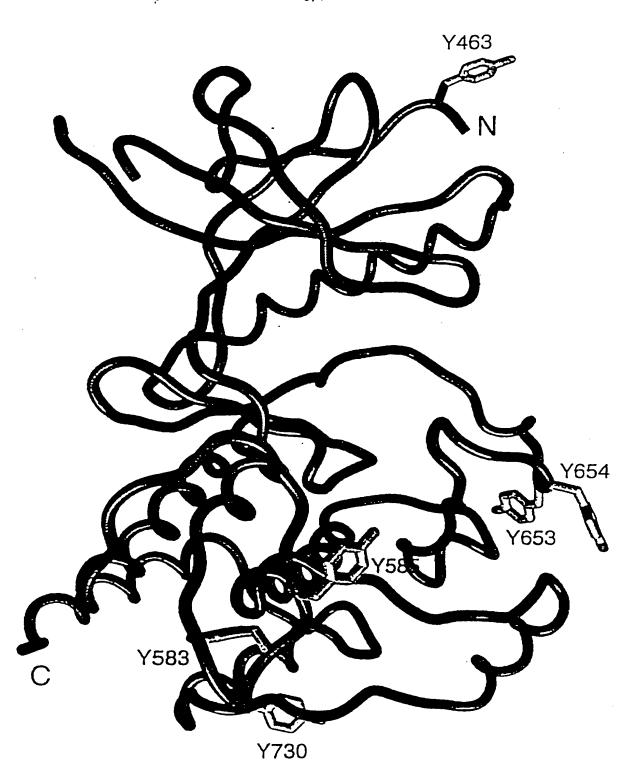


FIGURE 5

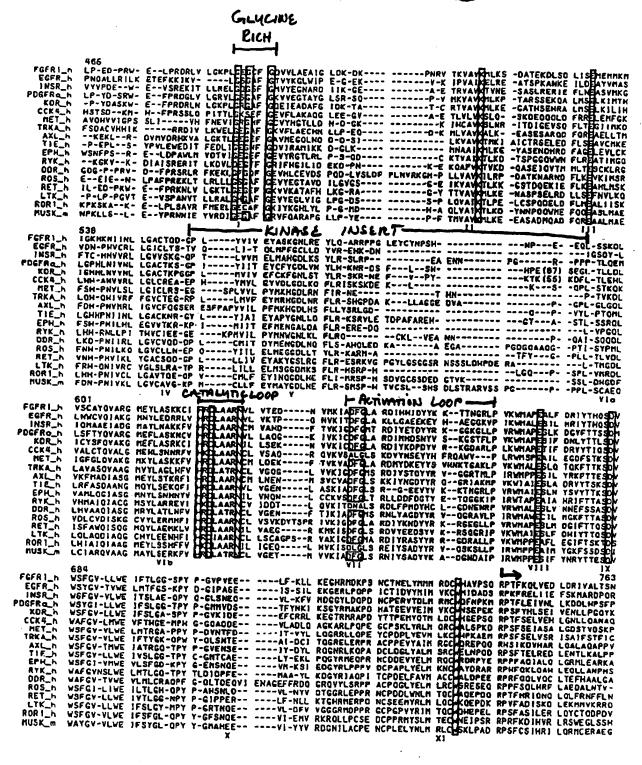


FIGURE 6A

FGFR1_h SRC_h BRK_h BTK_h CSK_h ZAP70_h FES_h FAK_h JAKI_h ACK_h	FEYRSGWAI N	MKELKILD-T	TEKEFEDYN	LGOY	RGNKVAV	KEIKNDA-TA	DLSDLISEME MMKMI-GKHK -EAFLO-E -QQMLQSE LQAMKKLRHE -QAFL-AE -QAFL-AE -KADTEEMHE ASVMTQLRHS -EEFLK-E KADTEEMHE AQIMHQLDNF LKAK-FLO-E GNHIAOLKKE IEILRNLYHE PEAMDOFIRE VNAMHSLDHR	<b>3</b> .
FGFR1_h SRC_h BRK_h CSK_h ABL_h ZAP7O_h FES_h FES_h JAK1_h ACK_h	KLYQLYAVVS HILALYAVVS KLYQLYGYCT NLYQLLGYIV NLYQLLGYIV YIYRLIGYCQ NIYRLIGYCT HIYKLIGYIT	-E-EP-IYIV VG-DP-VYII KQR-P-IFII EEKGG-LYIV REP-P-FYII AEALMLV -QKOP-IYIV ENPVWII	TEYMSKGSLL TELHAKGSLL TEYMANGSLY TEYMAKGSLY TEFHTYGNLL MEHAGGGPLH MELVQGGDFL MELCTLGELR	DFLKGET ELLROSD NYLRE-M OYLRECN KFLYGK TFLRTE SFLQVR		-EKYLPCYSEL -EKYLPVSEL -RHRFOTOOL -RSYLGGDCL -ROEVNAYYL -REEIPVSNY -GARLRYKTL -KYSLOLASOO	VSCAYGYARG MEYLASKKCI VDMAAQIASG MAYVERMNYV LDIAWQVAEG MCYLESQNYI LEMCKOVCEA MEYLESKOFL LKFSLDVCEA MEYLESKOFL LYMATQISSA MEYLEKKNFI AELLHQVSHG MKYLEEKNFV LQMVGDAAAG MEYLESKCI ILYAYQLSTA LAYLESKFV LKYAYQICKG MDYLGSRQYI SRYAVQVAEG MGYLESKRFI VID	
FGFR1_h SRC_h BRK_h BTK_h CSK_h ABL_h ZAP70_h FES_h FAK_h JAK1_h	HROLAARNOL HROLAARNOL HROLAARNOL HROLAARNOL	YSEDNYAKYS YGENHLYKYA LYNRHYAKIS	DFGLSKTT- DFGLSKLMT- DFGLSKALGA	-EASSTODTG GOTYTAHAGA DDSYYTARSA	-KLPYKWTAP -KFPIKWTAP GKVPLKWYAP RQYPYKWTAP GKLPIKWMAP ROSPYFWYAP RKYPFAWCAP	EALREKK-FS ESLAYNK-FS ECINFRK-FS	HQSDWSFGY LLWEIFTLGG IKSDWSFGI LLTELTTKGG TKSDWSFGI LLHEHFSRGG SKSDIWAFGY LHWEIYSLGK TKSDWSFGI LLWEIYSFGG IKSDWSFGG LLWEIATYGG SESDWSFGI LLWEITSLGA SASDWMFGY CHWEILHHGY IASDWSFGY TLHELLTYCG HASDIWMFGY TLWEHFTYGG	
FGFRI_h SRC_h BRK_h BTK_h CSK_h ABL_h ZAP70_h FES_h FAK_h JAKI_h ACK_h	V V S S	PYPGHYPYERFIPYPGIDPYKKHKPYPNLSPFQGYK KHIGPTHGOH	NREVLDQVER NHEAFLRYDA NSETAEHIAQ LKDVVPRVEK LSQVYELLEK GPEYMAFIE- NQQTREFVEK NNDVIGRIE-	-GYRMPCPHE -GYRMPCPHE -GLRLYRPHE -GYKMDAPDG -DYRMERPEG OGKRMECPPE -GGRLPCPPH NGERLPMPPN EGKRLPCPPN	CPPSVHKLHL ASEKYYTIHY CPPAVYEVMK CPEKYYELMR CPPELYALMS CPDAVFRLMT CPPEVYGLMR CPPEVYGLMR	TOTROPEOR SCHEKADER NCHLDAAHR ACIDWNPSOR OCH YKWEDR OCH YKWEDR KCHAYEPSRR KCHEFOPSNR	PTFKQLVEOL DRIVALTSNO PTFEYLQAFL EDYFTSTEPO PCFKALRERL SSFTSYENPT PTFKILLSNI LOVMOEES PSFLQLREQL EHIKTHELHL PSFAEIHQAF ETMFGESSIS PDFLTVEQRH RACYYSLASK PSFSTIYQEL QSIRKRHR PRFTELKAQL STILEEEKAQ TSFONLIEGFEALLK PTFVALROFL LEAQPTOMRA	

FIGURE 6B

f ,j





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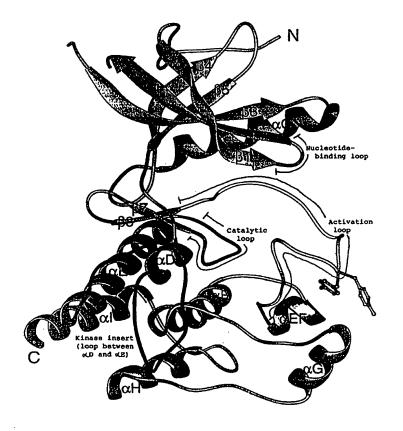
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(54) Title: CRYSTAL STRUCTURES OF A PROTEIN TYROSINE KINASE

#### (57) Abstract

The present invention relates to the three-dimensional structures of a protein tyrosine kinase optionally complexed with one or more compounds. The atomic coordinates that define the structures of the protein tyrosine kinase and any of the compounds bound to it are pertinent to methods for determining the three-dimensional structures of protein tyrosine kinases with unknown structure and to methods that identify modulators of protein tyrosine kinase functions.



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#### DESCRIPTION

#### CRYSTAL STRUCTURES OF A PROTEIN TYROSINE KINASE

5 <u>RELATED APPLICATIONS</u>

This application is related to U.S. Application Serial No. 08/701,191, by Mohammadi, et al., entitled "Crystals of the Tyrosine Kinase Domain of Non-Insulin Receptor Tyrosine Kinases," filed August 21, 1996 (Lyon & Lyon Docket No. 227/088) and U.S. Application Serial No. 60/034,168, by McMahon, et al., entitled "Crystal Structures of a Protein Tyrosine Kinase Complexed with Compounds of the Oxindolinone/Thiolindolinone Family," filed December 19, 1996 (Lyon & Lyon Docket No. 221/282), which are hereby incorporated herein by reference in their entirety including any drawings, tables, and figures.

# INTRODUCTION

The present invention relates to the three dimensional structures of protein kinases.

#### BACKGROUND OF THE INVENTION

The following description of the background of the invention is provided simply as an aid in understanding the invention and is not admitted to describe or constitute prior art to the invention.

Protein tyrosine kinases (PTKs) comprise a large and diverse class of enzymes (for a review, see Schlessinger and Ullrich, 1992, Neuron 9: 383-391). The PTK family contains multiple subfamilies, one of which

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is the fibroblast growth factor receptor (FGF-R) subfamily (for a review, see Givol and Yayon, 1992, FASEB J. 6 (15): 3362-3369).

All PTKs enzymatically transfer a high energy phosphate from adenosine triphosphate to a tyrosine residue in a target protein. These phosphorylation events regulate cellular phenomena in signal transduction processes. Cellular signal transduction processes contain multiple steps that convert an extracellular signal into an intracellular signal. intracellular signal is then converted into a cellular response. PTKs are components in many signal transduction processes. A PTK regulates the flow of a signal in a particular step in the process by phosphorylating a downstream molecule. The addition of a phosphate can either modulate the activity of the downstream molecule by turning it "on" or "off". Thus, aberrations in a particular PTK's activity can either cause overflow or underflow of the signal. Overflow of a signal can lead to such abnormalities as uncontrolled cell proliferation, which is representative of such disorders as cancer and angiogenesis.

Scientists in the biomedical community are searching for PTK inhibitors that down-regulate overflow signal transduction pathways. In particular, small molecule PTK inhibitors are sought that can traverse the cell membrane and not become hydrolyzed in acidic environments. These small molecule PTK inhibitors can be highly bioavailable and can be administered orally to patients.

Some small molecule PTK inhibitors have already

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been discovered. For example, bis(monocyclic), bicyclic or heterocyclic aryl compounds (PCT WO 92/20642), vinylene-azaindole derivatives (PCT WO 94/14808), 1-cyclopropyl-4-pyridyl-quinolones (U.S. Patent No. 5,330,992), styryl compounds (U.S. Patent No. 5,217,999), styryl-substituted pyridyl compounds (U.S. Patent No. 5,302,606), certain quinazoline derivatives (EP Application No. 0 566 266 A1), seleoindoles and selenides (PCT WO 94/03427), tricyclic polyhydroxylic compounds (PCT WO 92/21660), and benzylphosphonic acid compounds (PCT WO 91/15495) are described as PTK inhibitors.

Although many PTK inhibitors are known, many of these are not specific for PTK subfamilies and will therefore cause multiple side-effects as therapeutics. Compounds of the indolinone family, however, are specific for the FGFR subfamily and are non-hydrolyzable. WO 96/40116, "Indolinone Compounds for the Treatment of Disease," published December 19, 1996, inventors Tang et al. Although the use of X-ray crystallography has provided three dimensional structures of other PTKs, they are not complexed with PTK subfamily specific, hydrolysis resistant, small molecules.

Despite recent advances, the need remains in the art for crystallographic analysis of protein kinases, so that improved therapeutic molecules can be designed and synthesized.

# SUMMARY OF THE INVENTION

The present invention relates to the three

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dimensional structures of protein tyrosine kinases. The use of X-ray crystallography can define the three dimensional structure of protein tyrosine kinase at atomic resolution.

The three dimensional structures described herein elucidate specific interactions between protein tyrosine kinases and compounds bound to them. The coordinates that define the three dimensional structures of protein tyrosine kinases are useful for determining three dimensional structures of PTKs with unknown structure. In addition, the coordinates are also useful for designing and identifying modulators of protein tyrosine kinase function. These modulators are potentially useful as therapeutics for diseases, including (but limited to) cell proliferative diseases, such as cancer, angiogenesis, atherosclerosis, and arthritis.

Thus in a first aspect, the invention features a crystalline form of a polypeptide corresponding to the catalytic domain of a protein tyrosine kinase.

The term "crystalline form," in the context of the invention, is a crystal formed from an aqueous solution comprising a purified polypeptide corresponding to the catalytic domain of a PTK. A crystalline form of a protein tyrosine kinase is characterized as being capable of diffracting x-rays in a pattern defined by one of the crystal forms depicted in Blundel et al., 1976, Protein Crystallography, Academic Press. A crystalline form of a protein kinase is not characterized as being capable of diffracting x-rays in a pattern analogous to a crystalline form consisting of primarily salt or primarily a compound, for example.